



E-Abstract Book

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**53rd International Union of Pure & Applied Chemistry General Assembly (IUPAC 2025)
and 50th World Chemistry Congress (50WCC)**

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FROM COHERENCE IN PHOTOSYNTHESIS TO CHEMICAL QUANTUM INFORMATION SCIENCE

Gregory D. Scholes

Princeton University

Corresponding author: gscholes@princeton.edu

Abstract

The parallel and synergistic developments of atomic resolution structural information, new spectroscopic methods, their underpinning formalism, and the application of sophisticated theoretical methods have led to a step function change in our understanding of photosynthetic light harvesting. These new spectroscopic methods, in particular multidimensional spectroscopies, have enabled a transition from recording rates of processes to focusing on mechanism. Such studies indicated the possibility that advanced ultrafast techniques can give insights into the time evolution of the density matrix of the system. I will explain the story of how our understanding of these experiments evolved. We then ask, how might related developments enable advances in quantum information science? A defining characteristic of molecules is that they are intrinsically complex quantum systems with many degrees of freedom, exhibiting remarkable variety. Molecules, therefore, have different quantum properties than atomic systems, including solids. Our aim in chemical quantum information science (QIS) should then be to leverage these distinctions. This is where transformative advancements lie. I will outline and motivate the QIS “wish list” for chemistry that we described in a recent report.

THE EXCITING POTENTIAL OF AI FOR DRUG AND THERAPEUTIC DISCOVERY

David A. Winkler

Professor of Biochemistry & Chemistry, La Trobe Institute for Molecular Science, La Trobe University, Bundoora 3086, Australia; Professor of Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville 3052, Australia; Professor of Pharmacy, University of Nottingham, Nottingham NG7 2RD, UK
Corresponding author: D.winkler@latrobe.edu.au

Abstract

The current era has seen truly paradigm shifting scientific developments. We also know that the size of small molecule and materials spaces is for all practical purposes infinite, providing an inexhaustible supply of potential drugs and materials with valuable properties if we can find them. This recognition has seen a rapid increase in automation and robotics, allowing synthesis of new molecules and materials and measurement of properties orders of magnitude faster than before, generating massive databases of complex genetic, structural, chemical, property, and biological information.

The need to find ‘islands of chemical utility’ in an almost infinite palette of possibilities has seen the development of new data-driven machine learning methods (ML), like deep learning and large language models (LLMs), and an unprecedented increase in their applications. ML algorithms are universal approximators, prompting a parallel rise in their applications to most other aspects of modern life – medicine, finance, manufacturing, social media etc. we now have rapid and accurate quantum machine learning methods, generative methods that use trained machine learning models to suggest new molecules or materials with improved properties, accurate prediction of protein structures from sequence using AlphaFold and similar, the beginnings of general AI in LLMs like ChatGPT, massive ‘make on demand’ chemical libraries such as ZINC-22, nascent autonomous chemical discovery systems, and a rise in evolutionary AI methods for molecule and materials discovery.

This paper will discuss the drivers for these exciting developments and give examples where my collaborators and I have used AI and machine learning in biomaterials and regenerative medicine, drug design, energy materials and nanomaterials, cancer diagnostics, and corrosion control.

Keywords: Machine learning; drug design; artificial intelligence, materials discovery

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REALIZING CHEMISTRY'S PIVOTAL ROLE IN OUR SUSTAINABLE FUTURE

Peter G Mahaffy

The King's University and the King's Centre for Visualization in Science, Edmonton, Alberta, Canada

**Corresponding author: peter.mahaffy@kingsu.ca*

Abstract

Earth system science makes it increasingly clear that the scale and kinetics of anthropogenic transformation of matter have rapidly pushed the control variables for interconnected Earth systems closer to tipping points. The planetary sustainability and human security challenges facing our planet are so pressing that they require urgent attention by all of humanity through a convergence of disciplinary and cross-sectoral approaches. Chemistry, the science of transformation of matter, has a pivotal role to play in addressing the unintended consequences that arise from the large-scale material transformation by humans over the past fifty years. As the World Chemistry Congress begins, with a theme of "Chemistry for Our Sustainable Future," we can no longer see sustainability and the contributions of our central science as a goal, but rather an imperative.

The clock is ticking as we rapidly approach the target dates for meeting the UN Sustainable Development goals (2030) and the 2050 global energy net-zero agreements to mitigate the impact of humans on the energy balance of our planet. What re-imagining of chemistry education, research, and industry must we collectively embrace to practice chemistry responsibly in our rapidly changing world? IUPAC, through activities and structures that unite chemists and chemistry educators worldwide, plays a strategic role in guiding chemistry education, research and practice toward the emergence of sustainability. We will highlight IUPAC projects that:

- resource implementation of systems thinking in chemistry for sustainability with strands focused on chemistry as a sustainability science, formal chemistry education, and chemical industry; and
- introduce principles to guide chemists in the responsible practice of chemistry, informed by our pressing sustainability challenges and ethics, diversity, equity, and inclusion values. The project task group will formally launch the "IUPAC Guiding Principles of Responsible Chemistry" website at this Congress.

Keywords: sustainability, systems thinking, responsible chemistry, chemistry education



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BIOSENSORS WITHOUT FRONTIERS: NUCLEIC ACID TESTING IN LOW RESOURCE AREAS

Hall EAH*, Seevaratnam DJ, Roberts AL

Chemical Engineering and Biotechnology, University of Cambridge, CB3 0AS, UK

**Corresponding author: eah16@cam.ac.uk*

Abstract

The dynamics of infectious disease (ID) require fast accurate diagnosis for effective management and treatment. Without in-vitro diagnostics (IVDs) syndromic or presumptive actions are followed, where positive cases may go undetected in the community, or mistreated due to wrong diagnosis. This undermines effective clinical decision-making and disease containment. However, biosensor-diagnostics used in low and middle income countries (LMICs) usually have to be imported at high cost, making their use prohibitive.

The required biological reagents for a diagnostic are typically the largest proportion of the cost (50-95%). Taking a 'gene to diagnostic' approach, a rational design will be reported for a diagnostic platform that can be manufactured locally, with basic infrastructure. We use synthetic biology to design multifunctional fusion-enzymes for point-of-care diagnostics with locally resourced materials.

The platform is demonstrated for nucleic acid amplification tests (NAATs) requiring a DNA polymerase fusion protein which can be isolated on silica via a fused R5 silica-affinity peptide. Data from a clinical study of malaria are presented and the results discussed in comparison with qPCR, providing the first step towards low cost diagnostics in resource poor areas. This could deliver a sustained improvement in healthcare, while also developing the local economy.

SINGLE-ATOM CATALYSIS

Tao Zhang*

*^aState Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences,
Dalian, 116023, China*

**Corresponding author: taozhang@dicp.ac.cn*

Abstract

Single-atom catalysis has emerged as a new and possibly the most active frontier in heterogeneous catalysis. With the great potential for maximizing the atom efficiency and the well-defined active sites in a catalytic process, single-atom catalysts (SACs) have received incredibly increased attentions. Great advance has been achieved in the past few years in the preparation of highly efficient SACs, the exploration of new reactions, as well as the mechanism understanding of catalysis. In this lecture, I will introduce the fast progress of SACs and mainly focus on the research in my group to address some of the fundamental issues about single-atom catalysis, including the nature of the active sites in SACs, the essential role of coordination structure of single atoms, as well as the dynamics of SACs during reactions. Moreover, the significant opportunities and challenges in this new field of catalysis will be discussed.

PUSHING BOUNDARIES: INNOVATIONS IN ORGANOMETALLIC COMPLEXES AND CATALYSTS FOR ADVANCED CHEMICAL TRANSFORMATIONS

Zhaomin Hou

*Advanced Catalysis Research Group, RIKEN Center for Sustainable Resource Science,
2-1 Hirosawa, Wako, Saitama 351-0198, Japan*

*Organometallic Chemistry Laboratory, RIKEN Cluster for Pioneering Research,
2-1 Hirosawa, Wako, Saitama 351-0198, Japan*

Corresponding author: houz@riken.jp

Abstract

In this lecture, I would like to share our studies on the development of innovative organometallic complexes and catalysts, aiming at achieving unprecedented chemical transformations and advancing functional polymer synthesis. Representative examples include dinitrogen (N_2) activation and functionalization in well-defined multimetallic hydride frameworks, asymmetric C-H functionalization by organo rare-earth catalysts, and creating novel self-healing polymers by catalyst-controlled sequence regular polymerization and copolymerization of olefins and dienes. Our research underscores the crucial role of catalyst development in chemical synthesis. Looking ahead, exploring the potential of organometallic complexes and catalysts in diverse chemical transformations will continue pushing the frontiers of synthetic methodologies to meet the demands of sustainable and efficient chemical processes.

GREEN CHEMISTRY TOWARD LOW-SUGAR UNIVERSAL VACCINES AND GLYCOENGINEERED ANTIBODIES

Chi-Huey Wong

*Department of Chemistry, The Scripps Research Institute
La Jolla, CA 92037 and Genomics Research Center, Academia Sinica
Corresponding author: wong@scripps.edu*

Abstract

Glycosylation is a reaction used by Nature to modulate the structure and function of biomolecules. Most human viruses and cancer cells, for example, depend on the host glycosylation machinery to create a sugar coat on the cell surface to complete their life cycle and escape immune response. Understanding the role of cell surface glycans in viral infection, cancer progression and immune response requires easy access to this class of complex materials. This lecture will present our recent development of efficient and environmentally friendly chemoenzymatic methods for the synthesis of complex carbohydrates and glycoproteins and development of low-sugar universal vaccines and glycoengineered antibodies with improved Fc-mediated killing.

RETHINKING FLUORINE CHEMISTRY WITH GLOBAL CHALLENGES IN MIND

Véronique Gouverneur

University of Oxford, United Kingdom

Corresponding author: veronique.gouverneur@chem.ox.ac.uk

Abstract

The Gouverneur laboratory has developed new approaches for the synthesis of fluorochemicals for applications in the life and material sciences. This work has enhanced our fundamental understanding of alkali metal fluoride reactivity, and led to the invention of hydrogen bonding phase transfer catalysis (HBPTC), a new concept in organocatalysis opening new opportunities in organic chemistry. In this lecture, the discussion will focus on innovative approaches aimed at addressing the challenges currently facing the fluorochemical industry. A specific highlight is the demonstration that it is possible to convert naturally occurring fluorspar (CaF_2) into complex fluorochemicals applying a method that bypasses the necessity to manufacture hydrofluoric acid, a toxic and highly dangerous acid. Another recent advance is the design of a method for the destruction of PFAS coupled with fluorine recovery in the spirit of a circular fluorine economy.

ADVANCING THE FRONTIERS OF SEMICONDUCTING POLYMERS THROUGH PRECISION SYNTHESIS

Christine K. Luscombe

*pi-Conjugated Polymers Unit, Okinawa Institute of Science and Technology, 1919-1 Tancha, Onna-son, Okinawa,
904-0495, Japan*

Corresponding author: christine.luscombe@oist.jp

Abstract

Direct arylation polymerization (DAP) has gained significant attention for synthesizing conjugated polymers, offering advantages over conventional cross-coupling methods. DAP reduces organometallic waste and eliminates the need for prefunctionalization, thus enhancing atom economy. It generates benign by-products and requires only halogen-functionalization of one monomer. However, challenges in achieving selectivity and control during polymerization persist.

To address these issues, our group explored synergistic catalysis using Pd/Ag or Au/Ag combinations. This approach enables reactions previously unattainable with single catalysts. We initially focused on developing a controlled DAP to produce polymers with targeted molecular weights and low dispersities. Using dual catalysts, one for C-H activation and another for controlled polymerization, we demonstrated some living characteristics, albeit with low molecular weights.

We extended this work to donor-acceptor copolymer synthesis via cross dehydrogenative coupling (CDC). Unlike standard DAP, which couples C-Br and C-H groups, CDC involves C-H/C-H coupling, where selectivity is critical to avoid homocoupling products. Employing a Pd/Ag cocatalyst system, we achieved high selectivity, producing high molecular weight polymers with minimal defects. The second chain-extension cross-coupling occurred at least an order of magnitude faster than the first coupling or homocoupling side reactions. DFT calculations revealed that the enhanced rate of cross-coupling in the second step stems from a strong Pd-thiophene interaction, which lowers the energy barrier for Pd-mediated C-H activation. These findings not only improve polymerization processes but also have broader applications in synthesizing complex molecules where C-H bond activation is challenging.

DESIGN AND SYNTHESIS OF NANOMATERIALS FOR BIOMEDICAL AND ENERGY APPLICATIONS

Jackie Y. Ying

*Department of Bioengineering and Nanomedicine, King Faisal Specialist Hospital & Research Centre Riyadh,
Saudi Arabia*

Corresponding author: jyying66@gmail.com

Abstract

Nanostructured materials can be designed with sophisticated features to fulfill the complex requirements of advanced material applications. Our laboratory has developed organic and inorganic nanoparticles and nanocomposites for advanced drug delivery, antimicrobial, stem cell culture, and tissue engineering applications. In addition, we have nanofabricated microfluidic systems for drug screening, *in vitro* toxicology, and diagnostic applications. The nanosystems allow for the rapid and automated processing of drug candidates and clinical samples in tiny volumes, greatly facilitating drug testing, genotyping assays, infectious disease detection, point-of-care monitoring, as well as cancer diagnosis and prognosis.

We have also synthesized metallic, metal oxide and semiconducting nanoclusters, nanocrystals and nanosheets of controlled dimensions and morphology. The nano-sized building blocks are used to create multifunctional systems with excellent dispersion and unique properties. Nanoporous materials of a variety of metal oxide and organic backbone have also been created with high surface areas and well-defined porosities. These nanostructured materials are successfully tailored towards energy and sustainability applications.

CINEMATIC CHEMISTRY: THE JOURNEY OF ELECTRON MICROSCOPY FROM ORGANIC SYNTHESIS TO MOLECULAR STATISTICS

Eiichi Nakamura

The University of Tokyo, Japan

Nankai University, China

Corresponding author: nakamura@chem.s.u-tokyo.ac.jp

Abstract

Recent technological innovations in electron microscopy, such as aberration correctors, high-speed imaging cameras, and continuous sample rotation, have ushered in a new era where we can, for the first time, analyze the behavior of individual molecules. In this lecture, I will introduce the new paradigm of “cinematic chemistry,” which has emerged from the single-molecule atomic-resolution time-resolved electron microscopy (SMART-TEM). I will use examples from single-molecule thermodynamics and kinetics based on ultra-fast imaging of individual molecules and reaction events, *in situ* structural and statistical analysis of crystal growth, and the mechanisms behind organic crystal disorder during electron diffraction experiments that has long confused electron microscopists. Our recent study has shown that the kinetics of electron diffraction peak decay provides quantitative information about the degree of freedom of the molecules in a crystal.

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CONTINUOUS MOVEMENT OF CARBON ATOMS IN ORGANIC MOLECULES: MERRY-GO-ROUND REACTION

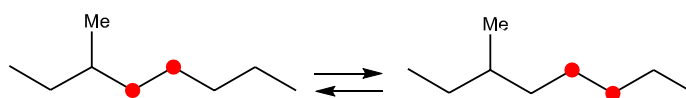
Tamotsu Takahashi

Institute for Catalysis, Hokkaido University, Sapporo, Japan

Corresponding author: tamotsu@cat.hokudai.ac.jp

Abstract

Continuous movement of carbon atoms in organic molecules is a challenging target in chemistry. I proposed a new concept to achieve such movement using equilibrium of two organic molecules where positions of carbon atoms are not the same. Even though the mechanism of the equilibrium is not clear, more stable compound is formed among the molecules in the equilibrium by moving of the target carbon atoms in the organic molecules.



New concept for the movement of carbon atoms in organic molecules.
More stable compound is formed in the equilibrium by movement of carbon of carbon atoms.

I applied this new concept for dihydroindenyl moiety on titanium, and I could developed that two red carbons at the bridge-head positions of dihydroindenyl moved around the six-membered ring. I named this reaction, “Merry-Go-Round Reaction”.

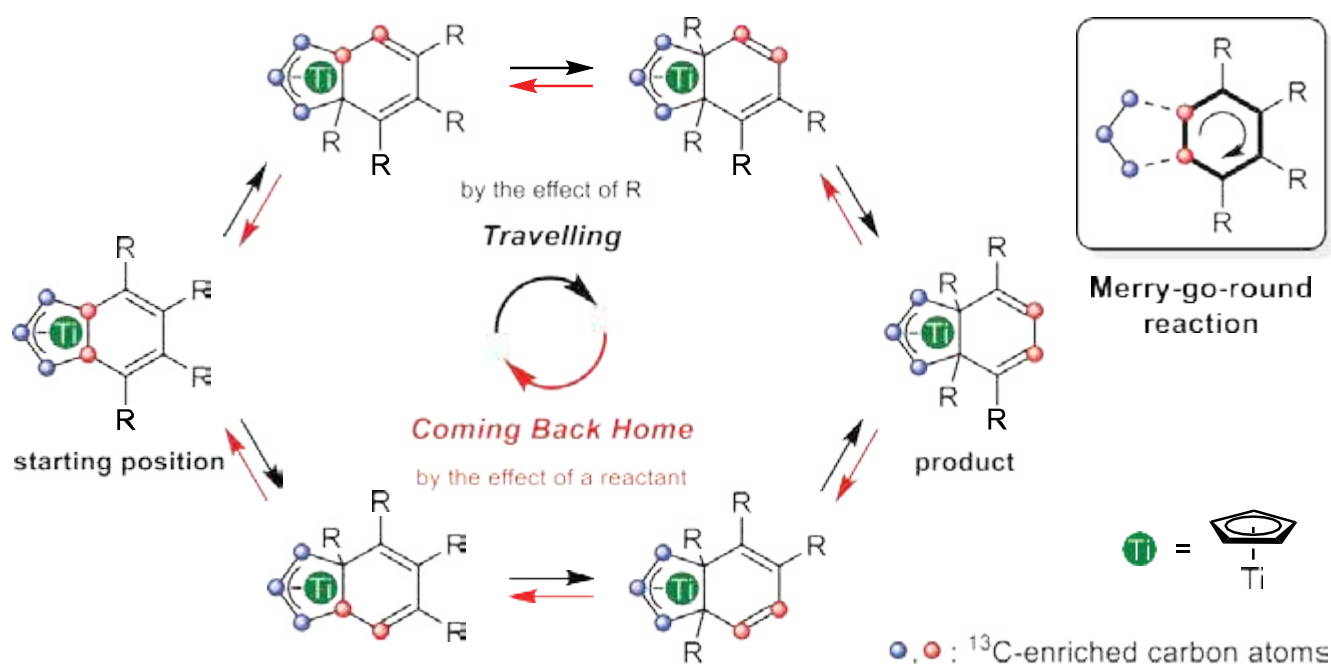


Figure. Travelling of carbon atoms in organic molecules **Merry-Go-Round Reaction**

g-xTB: DFT ACCURACY AT TIGHT-BINDING SPEED

Stefan Grimme

*Mulliken Center for Theoretical Chemistry, Clausius Institute for Physical and Theoretical Chemistry,
University of Bonn, Berlingstraße 4, 53115 Bonn, Germany
Corresponding author: jwt@kncv.nl*

Abstract

I will present our third-generation tight-binding electronic structure model g-xTB (g=general) for general chemistry applications. This includes non-local Fock-exchange as well as other new, many-center Hamiltonian terms (e.g., atomic correction potentials, ACP). Another important new ingredient is the adaptive q-vSZP minimal AO basis set[1] which provides in typical DFT applications results of about or better than DZ quality. The "breathing" of the AOs in the molecular environment is parameterized efficiently by on-the-fly computed effective atomic charges obtained by a new EEQ-bond-capacitor charge model[2] and coordination numbers.

g-xTB aims at general purpose applicability and more closely approaches DFT accuracy (actually ω B97M-V/aTZ[3]) than previous semi-empirical methods at only slightly increased computational cost (factor of 1.5 compared to GFN2-xTB). It will be consistently available for all elements $Z=1-103$ with f-electrons included for lanthanides/actinides. The talk gives a fresh look at the underlying TB theory as well as extensive benchmarking on a wide range of standard thermochemistry sets.

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MESOSTRUCTURED MATERIALS DRIVING INNOVATIONS IN CLEAN ENERGY AND ENVIRONMENTAL SUSTAINABILITY

Joon Ching Juan

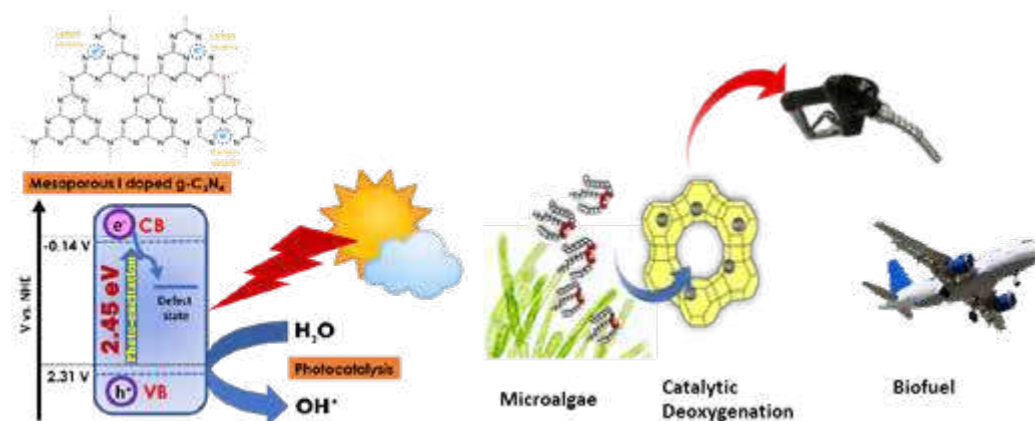
*Nanotechnology and Catalysis Research Center (NANOCAT), Universiti Malaya,
50603 Kuala Lumpur, Malaysia*

Corresponding author: jcjuan@um.edu.my (Juan JC)

Abstract

Rapid economic growth has given rise to two critical global challenges, namely environmental pollution and the need for sustainable energy. Among these, water contamination caused by diverse persistence organic pollutants in wastewater poses serious threats to both human health and aquatic ecosystems. At the same time, heavy reliance on fossil fuels has led to excessive greenhouse gas emissions. In line with the United Nations Sustainable Development Goals (SDGs) 6 (Clean Water and Sanitation) and 7 (Affordable and Clean Energy), there is an urgent need to explore new pathways that support economic advancement while ensuring sustainability. Mesostructured materials characterized by their high surface area and porosity, offer promising potential to meet these goals. Our research is dedicated to the development and structural engineering of advanced mesoporous materials, with a focus on mesoporous titania, hexagonal mesoporous silica, hierarchical zeolites, molybdenum disulfide, and mesoporous graphitic carbon nitride. These tailored mesoporous catalysts have shown remarkable hydrogen-free deoxygenation activity for biofuel production with over 85% yield. The results highlight that surface area, porosity, and catalytic acidity play key roles in enhancing deoxygenation activity. In addition to a high surface area, tailoring structural imperfections in mesoporous photocatalysts, such as introducing oxygen vacancies, creates a synergistic effect that dramatically improves photocatalytic activity. We are among the pioneers in applying mesoporous materials for photocatalytic wastewater treatment and the hydrogen-free deoxygenation of non-edible oils into biofuels. The exceptional catalytic efficiency of mesostructured arises from the synergistic contributions of large surface area, high porosity, reduced electron-hole recombination, narrowed band gaps, and intrinsic acidity. Our innovative strategy has opened a new direction for engineering mesoporous materials with targeted modifications to effectively deliver clean water and sustainable energy solutions.

Keywords: Mesoporous, catalysis, deoxygenation, photocatalysis, biofuel



Acknowledgement

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RETICULAR CHEMISTRY, CLIMATE, AI

Omar M. Yaghi

Department of Chemistry, Bakar Institute of Digital Materials for the Planet, University of California, Berkeley

**Corresponding author: yaghi@berkeley.edu*

Abstract

The clean air, clean energy, and clean water challenges facing our planet today impact our health, wealth, happiness, and future. These three stresses present difficult science and engineering problems requiring, the selective capture of small molecules (e.g. hydrogen, methane, carbon dioxide, and water). Our ability to capture, store, manipulate, and harness the power of these molecules in an efficient and economical manner is paramount to our success in building a sustainable future. The emerging field of reticular chemistry has yielded extensive classes of ultra-porous metal-organic frameworks and covalent organic frameworks. The flexibility with which these materials can be made, modified, and scaled bodes well for their integration into devices and providing robust solutions to these challenges. In this presentation, I will highlight how reticular chemistry has led us to make frameworks for carbon capture from air and flue gas, as well as for harvesting water from air to produce drinking water in various parts of the world regardless of temperature and humidity levels. Our efforts in taking this technology from the laboratory to the field including the design and engineering of prototypes and applying AI tools to speed up discovery will be discussed and the results presented.

THE STOCKHOLM DECLARATION ON CHEMISTRY FOR THE FUTURE

Paul T. Anastas

*Center for Green Chemistry and Green Engineering
Yale University*

**Corresponding author: paul.anastas@yale.edu*

Abstract

On May 23, 2025, The Stockholm Declaration on Chemistry for the Future was first presented to the public. This declaration is a list of imperatives on how the power of chemistry must be implemented at scale for the benefit of people, prosperity, and the planet. This declaration was the work of scientists and engineers from around the world who convened at the “Nobel Symposium on Chemistry for Sustainability: Fundamental Advances”. One of the most important sentences in the declaration is “sustainability without innovation would be impossible and innovation without sustainability would be ruinous.”

The declaration is a call to action to build on and continue the brilliant inventions and innovations of scientists and engineers **AND** to engage the broader public in the critical work of education, investment, policymaking, communication, and beyond to ensure that the best of our chemical technologies are actually implemented to improve life for today’s society and tomorrow’s generations.

The Stockholm Declaration on Chemistry for the Future is open to all individuals, organizations, institutions, businesses, companies, and governments to sign it and join in the efforts to implement chemistry that results in a better world.

All are invited to sign the Declaration at the weblink below:

<https://www.stockholm-declaration.org>



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PUTTING THE SOLVENT IN THE SPOTLIGHT

Martina Havenith

Department of Physical Chemistry II, Ruhr University Bochum, Germany

**Corresponding author: martina.havenith@rub.de*

Abstract

Exploring the unique role of water for life is one of the top future challenges in chemistry. Whether fast protein motion and solvent dynamics are correlated at the very heart of enzymatic reactions is still under heated debate. The underlying molecular mechanism of enthalpy-entropy (H/S) compensation in protein-ligand binding remains controversial. Systematic studies under steady state conditions revealed that differences in the structure and thermodynamic properties of the waters surrounding the bound ligands are an important contributor to the observed H/S compensation. These hydration free energies are dictated by a subtle balance of hydrophobic and hydrophilic interactions. Calorimetry served as a powerful biophysical tool by measuring changes in thermodynamic state variables, but it is restricted to measurements in equilibrium and in macroscopic samples. THz calorimetry is a novel spectroscopic approach, which allows to deduce hydration free entropy and enthalpy based on spectroscopic observables. Thereby, we can probe reach time resolutions of up to picoseconds and probe inhomogeneous samples. By probing the low frequency range which is most sensitive to the intermolecular interactions (100–600 cm⁻¹), we established a direct correlation between spectroscopic observables and local contributions to the solvation free energy. Liquid-liquid phase separation (LLPS) describes the reversible compartmentalization of protein solutions into a protein-rich and a dilute phase; the former one being a local hotspot for neurotoxic aggregation in case of Alzheimer or Huntington disease. Using THz calorimetry, we observe how LLPS can be tuned by changes in hydration entropy and enthalpy. This allows to unravel two underlying molecular mechanism, which drive this process: The release of “Cavity-wrap” water hydrating hydrophobic patches during LLPS yielding an increase in entropy. In contrast, “Bound” water hydrating hydrophilic patches is retained. This process is enthalpically favorable. Both contributions favor protein aggregation in liquid droplets. A fundamental understanding of these processes is a prerequisite for tuning of LLPS.

Keywords: THz spectroscopy, THz calorimetry, Water, Liquid-liquid phase separation (LLPS)

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NANOENGINEERING CATALYSTS FOR BIOREFINING

Karen Wilson^{a,*}

^a*School of Environment & Science, Griffith University, Gold Coast Campus, Queensland, Australia.*

^{*}*Corresponding author: karen.wilson6@griffith.edu.au; k.wilson1971@gmail.com*

Abstract

The quest for sustainable technologies to meet the food, energy and material challenges of this century is a key driver for the design of next-generation catalysts and industrial chemical processes. Control over the rate and pathway of associated chemical transformations represents the Holy Grail for catalysis. The rational design of heterogeneous catalysts with optimal performance heavily relies on a detailed understanding of atomic and molecular interactions and associated reactions at solid surfaces, for which in situ and operando studies can offer unparalleled insight.

The design of new heterogeneous catalysts tailored to meet the increasingly stringent demands of sustainable processes requires consideration of both the macroscopic physico-chemical properties of new materials, and a microscopic understanding of the fundamental interactions between the catalyst surface and the reactants/products. This presentation will highlight how advances in inorganic synthesis, underpinned by nanoscale materials visualisation and molecular level insight into dynamic surface chemistry probed through in-situ time-resolved spectroscopies can unlock new high-performance catalysts. A particular focus will be how nanoengineering support architecture and nanoparticle morphology can overcome the scientific and engineering barriers to the conversion of sustainable feedstocks to platform chemicals, and monomers for renewable polymers.

Keywords: Biorefining; Operando spectroscopy; Catalysis; Sustainable Chemistry

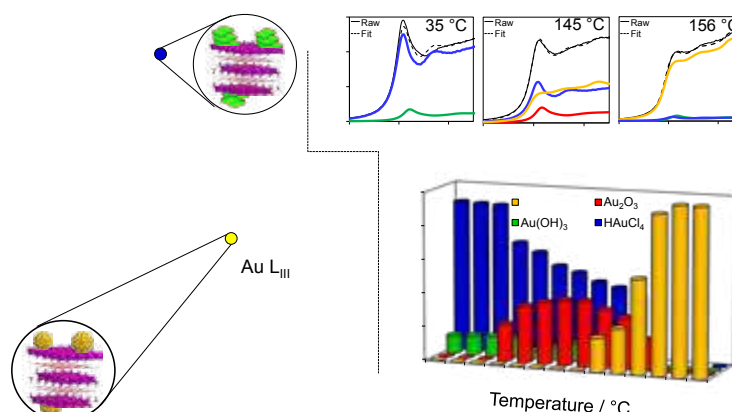


Fig. 1 In-situ XAS reveals how Au/LDH catalysts used for the synthesis of 2,5-furandicarboxylic acid evolve during thermal processing.

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DOING CHEMISTRY SUSTAINABLY

Michael Spencer, Michael Stevens, Jamie Hicks, Anthony Hill, Brett Schwartz, Darcy Williams, Andrew White, Rashid Javaid, Lara Malins, Michael Hill, Laura Dan, Alison Rodger*

Research School of Chemistry, The Australian National University, ACT 2603, Australia

**Corresponding author: alison.rodger@anu.edu.au*

Abstract

Introduction: The world is made of molecules and materials, so chemistry is a key part of addressing all of the challenges the world faces. However, traditional ways of doing chemistry are not always sustainable, as well as being expensive. In 2024 the Research School of Chemistry at The Australian National University spent 20% of its non-staff operational budget on waste disposal. In addition to the direct cost of disposal, there is also the carbon footprint of the incineration of the waste, the inconvenience of collection and storage of waste, and the need to buy large amounts of solvent for the next experiments.

Objective: We have therefore embarked on a journey to establish ways of *doing* chemistry more sustainably. We have begun to think of much of our chemistry in terms of the mantra: “reduce – reuse – recycle”.

Methods: This includes more efficient, less wasteful methods of synthesis (electrochemical, flow and ball mill) and purification, reuse of solvents, and easy-to-do waste solvent recycling.

Results and conclusions: We will report some of our data on how successful (or otherwise) we have been, where the quick wins are, and where we are still challenged to make progress. So far, we have reduced our waste solvent disposal collections to 50% of the 2024 number.

Keywords:

Sustainability, Molecules, Reduce, Reuse, Recycle

Graphic / Image



A solvent recycling system.

BRIDGING THEORY AND EXPERIMENT: TOWARDS REALISTIC MODELING OF COMPLEX SYSTEMS

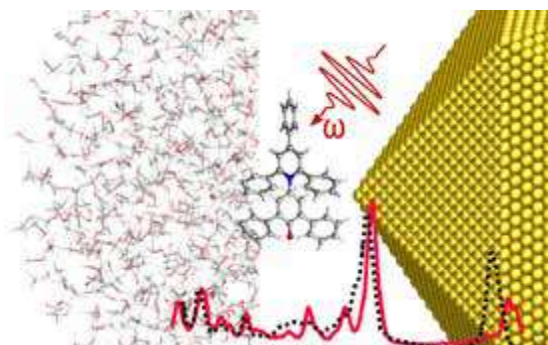
Tommaso Giovannini^{a,*}*Department of Physics, University of Rome Tor Vergata, Rome, Italy**Corresponding author: tommaso.giovannini@uniroma2.it

Abstract

The theoretical description of large molecular systems in the condensed phase at a high level of accuracy is particularly challenging, due to the large number of degrees of freedom (both electronic and nuclear) that must be properly accounted for. Such a chemical complexity typically arises in molecular systems in solution or interacting with a biological matrix, and it is even more pronounced when they are adsorbed on metal nanostructures supporting plasmon excitations – the physical mechanism underlying surface-enhanced spectroscopies, such as Surface-Enhanced Raman Scattering (SERS). From a theoretical perspective, these systems can be addressed within a unified framework based on the partitioning of the total system into smaller, interacting subsystems, with specific focus on the target system of interest [1-3]. The resulting focused models have been proven to be valuable tools for bridging the gap between theory and experiment [1-3].

In this talk, I will present and discuss recent developments in multiscale quantum mechanical (QM)/classical methodologies specifically developed to accurately describe complex molecular systems interacting with an external environment [3-6]. Various applications, ranging from chromophores in solution [3-5] to molecular systems interacting with plasmonic substrates (SERS) [6], will be discussed, illustrating the reliability and robustness of the methods through direct comparison with experimental data [3-8].

Keywords: Multiscale Modeling; QM/Classical; Condensed phase; Plasmonics; SERS; Solutions



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SOLVATION SHIFTS THE BAND-EDGE POSITION OF COLLOIDAL QUANTUM DOTS BY NEARLY 1 eV

Yan B. Vogel^{a,b,*}, Michelle L. Coote^c, Arjan J. Houtepen^b

^a*Institute of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland*

^b*Department of Chemical Engineering, Delft University of Technology, Van der Maasweg 9, 2629 HZ Delft, The Netherlands*

^c*Institute for Nanoscale Science and Technology, College of Science and Engineering, Flinders University, Bedford Park, South Australia 5042, Australia*

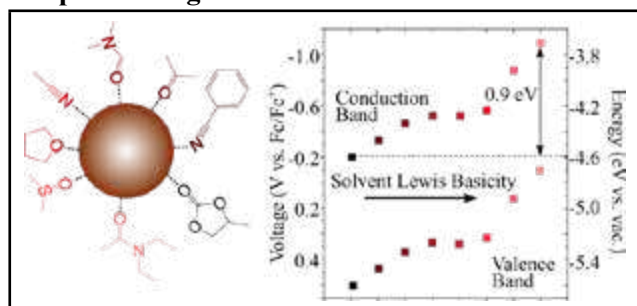
*Corresponding author: yvogel@ethz.ch

Abstract

The optoelectronic properties of colloidal quantum dots (cQDs) depend critically on the absolute energy of the conduction and valence band edges. It is well-known these band-edge energies are sensitive to the ligands on the cQD surface, but it is much less clear how they depend on other experimental conditions, like solvation. Here we experimentally determine the band-edge positions of thin films of PbS and ZnO cQDs via spectroelectrochemical measurements.¹ To achieve this, we first carefully evaluate and optimize the electrochemical injection of electrons and holes into PbS cQDs. This results in electrochemically fully reversible electron injection with >8 electrons per PbS cQDs, allowing the quantitative determination of the conduction band energy for PbS cQDs with various diameters and surface compositions. Surprisingly we find that the band edge energies shift by nearly 1 eV in the presence of different solvents, a result that also holds true for ZnO cQDs. Complexation and partial charge transfer between solvent and surface ions are responsible for this large effect of the solvent on the band edge energy. The trend in the energy shift matches the results of density functional theory calculations in explicit solvents and scales with the energy of complexation between surface cations and solvents. As a first approximation, the solvent Lewis basicity can be used as a good descriptor to predict the shift of the conduction and valence band edges of solvated cQDs.

Keywords: Quantum dots, semiconductor nanomaterials, electrochemistry, optoelectronics, spectroelectrochemistry

Graphic / Image



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REDEFINING PROTON AFFINITY FOR HETERONUCLEAR MOLECULAR SPECIES: QUANTUM CHEMICAL INSIGHTS

Emmanuel E. Etim^{a,*}, John Shinggu^a, Humphrey Samuel^a, Bulus Bako^a, Levie Mweene^b

^aDepartment of Chemical Sciences, Federal University, Wukari, Taraba State, Nigeria

^bDepartment of Earth Resources and Environmental Engineering, Hanyang University, Seoul - 04763, Republic of Korea

*Corresponding author: emmaetim@gmail.com

Abstract

One of the main problems with experimental methods for detecting proton affinity (PA) is that they cannot perform site-specific protonation. For heteronuclear molecular species that have two or more protonation sites, the experimental PA measurement only yields a single PA value for each molecular species, with no information on the protonation site. Using various quantum chemical calculation techniques, various heteronuclear molecular species with two to four protonation sites (with known experimental proton affinity values) were subjected to site-specific protonation in order to characterize the trends of the PA corresponding to the experimentally measured PA values for each heteronuclear molecular species. The results showed additional trends that correspond to the measured PA values, going beyond the widely held belief that the proton moves to the place of the highest electron density during protonation. These tendencies included the proton moving to the site of the lowest electron density. Redefining proton affinity for heteronuclear molecular species is strongly suggested by the many patterns that have been seen. Besides these tendencies, we also found some molecular species that showed significant differences between the actual and computed PA values using various approaches, suggesting that the stated experimental values might be inaccurate. These observations will be presented.

Keywords: Proton affinity, binding sites, heteronuclear species,

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THE INTERPLAY OF LIPID BILAYER FORCES AND ELASTICITY. THE BILAYER RESPONSE TO SMALL MOLECULE SOLVATION

Adriana Štuncová*

*Department of Polymers for Electronics and Photonics, Institute of Macromolecular Chemistry,
Czech Academy of Sciences, Prague 162 00, Czech Republic.*

**Corresponding author: stuncova@imc.cas.cz*

Abstract

Lipid hydrocarbon chains that are organized in a bilayer are not isolated and the rotation about their single carbon-carbon bonds is restricted due to intermolecular interactions (repulsive excluded-volume interactions, van der Waals interactions, and the surface terms – hydrophobic, electrostatic and hydration interactions). The ordering of the hydrocarbon chains can be evaluated by the use of the average deuterium order parameter as obtained from NMR spectroscopy.

It will be shown in this work, that two different approaches can be used to obtain the same mathematical description of lipid bilayer structure (*i.e.* the average area per hydrocarbon chain and properties derived from it) as a function of order parameter.¹ The agreement between the two approaches implies that the order parameter is, *i.a.*, a representation of the balance established between intra- and interbilayer forces (or pressures), while the model relates these forces to bilayer elastic properties. This model is a continuation of previous models relating the order parameter and the average chain geometry, and also of previous empirical models that related experimental values of determined from NMR spectroscopy, and the inverse average area per chain determined by X-ray diffraction.

The proposed model is applied to 1,2-dimyristoyl-*sn*-glycero-3-phosphatidylcholine (DMPC)/water bilayers to understand their response to solvation of a small amphiphilic molecule benzyl alcohol. Various binding sites are identified to exist within the bilayer – benzyl alcohol molecules partition between these sites, this equilibrium is dynamic and hydration-dependent. An observation is made that solubilization of benzyl alcohol molecules is terminated when the DMPC chains adopt certain limiting values of the order parameter throughout the chain. Such limit to the hydrocarbon chain disordering most likely reflects a more general property – the chain adopts the limiting chain order profile when the solute-bilayer system still exists as a single phase, just before the solute phase-separates.

Keywords: lipid bilayer, chain area, order parameter, solid-state NMR, X-ray, benzyl alcohol

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MODULATING MASS TRANSPORT UNDER CONFINEMENT VIA STRUCTURAL AND INTERFACIAL DESIGNS

Ningran Wu^{a,b}, Luda Wang^{a,b*}

^a Academy for Advanced Interdisciplinary Studies, Peking University, Beijing, 100871.

^b Beijing Graphene Institute, Beijing, 100095.

*Corresponding author: luda.wang@pku.edu.cn

Abstract

Mass transport under nanoconfinement differs significantly from that in the bulk counterpart. Understanding the mechanism can help us design efficient mass transport pathways and promote related applications. We employ biomimetic 2D material nanopores as ion and water pathways, and systematically investigated their underlying mechanisms. Intrinsic material properties—such as grain boundaries, surface roughness, and tunable functional groups—are leveraged to modulate transport behavior, with applications including ion separation, nanofluidic sensing, and energy conversions.

Proton exchange membrane fuel cells, as a zero-carbon method of direct conversion from chemical energy to electrical energy, have an expected energy utilization rate exceeding 60%. Mass transfer loss accounts for over 70% of the total voltage drop, severely affecting the output power of the fuel cell. Due to the slippage of water on the surface of graphene and inside carbon nanotubes, rapid water transport might promote transport in the microporous layer of the fuel cell. We used a graphene-doped microporous layer and achieve a peak output power of 1.1 W cm⁻². Electrochemical impedance spectroscopy characterization found that the high output power is due to the reduction of ohmic loss and mass transfer loss, which decreased by 80% compared with the traditional carbon black-based microporous layer. Our work bridges the gap between nanoscale transport principles and macroscale device engineering, paving the way for high-efficiency energy systems using nano-confinement architectures.

Keywords: 2D materials; interface; proton exchange membrane fuel cells; microporous layer; water and gas transport

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QUADRUPOLEAR-DRIVEN DONOR-ACCEPTOR π -SYSTEMS: TUNING THE ORDER-DEPENDENT PROPERTIES OF OPTOELECTRONIC BIOMOLECULAR COASSEMBLIES

Sheng Wei Tang^{a,b}, Herdeline Ann M. Ardoña^{a,b,c,d*}

^a Department of Chemistry, School of Physical Sciences, University of California, Irvine.

^b Department of Chemical and Biomolecular Engineering, Samueli School of Engineering, University of California, Irvine.

^c Department of Biomedical Engineering, Samueli School of Engineering, University of California, Irvine.

^d Sue and Bill Gross Stem Cell Research Center, University of California, Irvine.

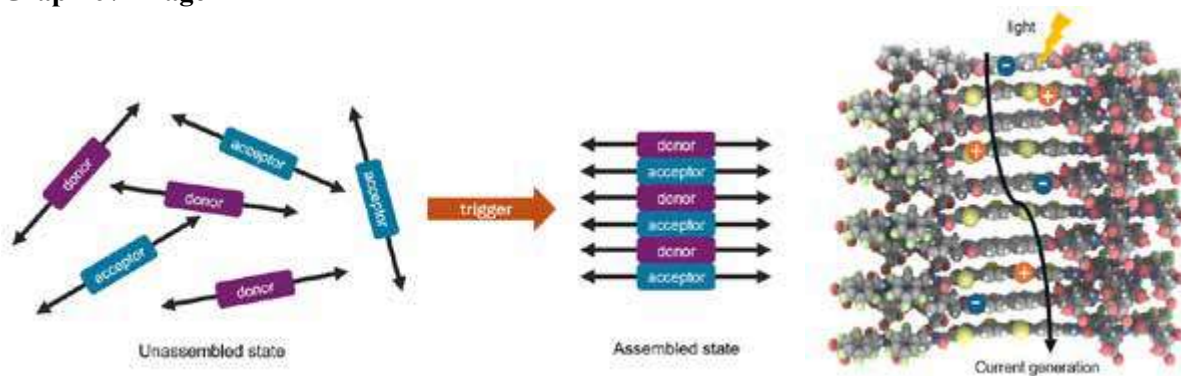
*Corresponding author: hardona@uci.edu

Abstract

Inspired by light-harvesting complexes found in Nature, peptide-based donor-acceptor materials have been studied and adapted to achieve desirable energy transfer properties due to its biocompatibility and tunability to funnel energy into its desirable state. Its electronic properties are highly dependent on the arrangement of π -conjugated systems at the molecular level.^{1,2} In prior studies, we have demonstrated that photophysical properties of conductive peptide materials can be tuned via sequence engineering and sequence charge complementarity.^{3,4} Here, we explore the impact of quadrupolar interactions by inserting halogenated point mutations in the molecular design of either the donor or acceptor component. Based on the initial solution conditions where the donor and acceptor units are subjected, we hypothesize that the one- and two-dimensional donor-acceptor interaction between the electron-rich and electron poor aromatics can be controlled by quadrupolar effects, which could in turn tune the photoinduced charge transfer properties of the self-assembled nanostructures. Herein, we focus on discussing the insights of different photophysical outcomes between the non-halogenated and halogenated assembly.

Keywords: peptide self-assembly, donor-acceptor systems, π - π stacking, charge transfer properties

Graphic / Image



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NUCLEASE-INDUCED STEPWISE PHOTODROPPING (NISP) TO PRECISELY INVESTIGATE SINGLE-STRANDED DNA DEGRADATION BEHAVIORS OF EXONUCLEASES AND ENDONUCLEASES

Hsiu-Fang Fan^{a,*}

^a Institute of Medical Science and Technology, National Sun Yat-sen University, Taiwan

^b Department of Chemistry, National Sun Yat-sen University, Taiwan

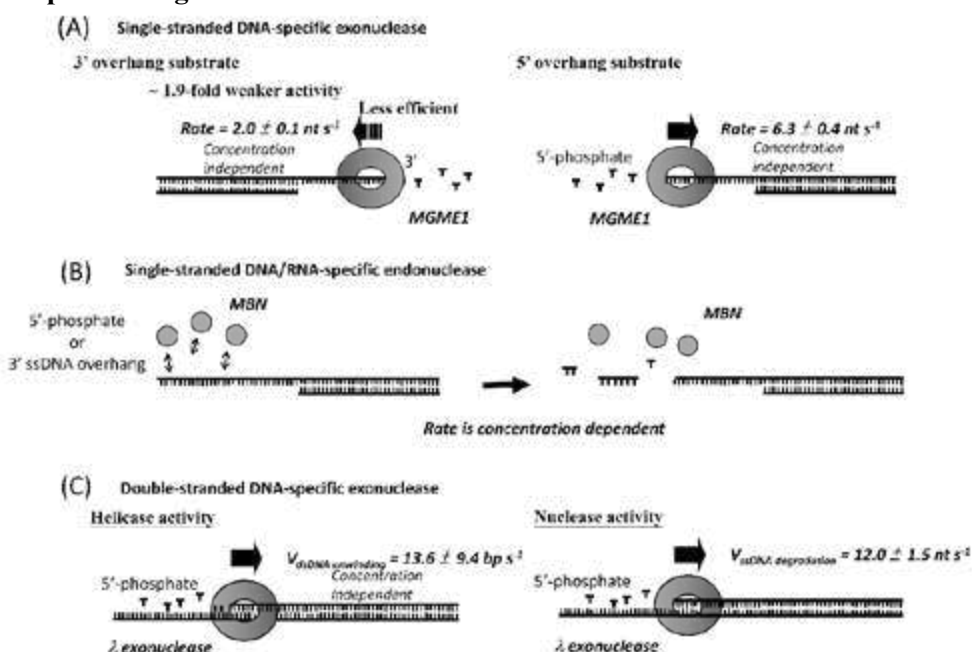
*Corresponding author: Bendyfan@imst.nsysu.edu.tw

Abstract

In this study, we utilized a fluorescence-based single-molecule technique, nuclease-induced stepwise photodropping (NISP), to monitor DNA degradation in real time. We applied NISP to analyze the activity of mitochondrial genome maintenance exonuclease 1 (MGME1), a single-stranded DNA (ssDNA)-specific exonuclease; Mung bean nuclease (MBN), a single-strand-specific endonuclease; and λ -exonuclease, which targets double-stranded (dsDNA) substrates. Our findings demonstrate NISP's ability to precisely and reliably quantify ssDNA degradation mediated by both exonucleases and endonucleases. This study establishes NISP as an effective tool for investigating the degradation dynamics of nucleases at the single-molecule level.

Keywords: (Nuclease-induced stepwise photodropping (NISP), single-strand-specific nuclease, MGME1, mung bean nuclease (MBN), λ exonuclease)

Graphic / Image



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LEAD HALIDE PEROVSKITES FOR ENERGY APPLICATIONS: STRUCTURAL COMPLEXITY AND DYNAMICS REVEALED BY SOLID STATE NMR

Elisa Carignani^{a,*}, Noemi Landi^a, Elisa Della Latta^b, Andrea Scarperi^b, Silvia Borsacchi^a, Lucia Calucci^a, Marco Geppi^b, Francesca Martini^b

^a*Institute for the Chemistry of OrganoMetallic Compounds, National Research Council, CNR-ICCOM, via G. Moruzzi 1, 56124 Pisa, Italy*

^b*Department of Chemistry and Industrial Chemistry, University of Pisa, via G. Moruzzi 13, 56124 Pisa, Italy*

**Corresponding author: elisa.carignani@cnr.it*

Abstract

Lead Halide Perovskites (LHPs), of general formula $APbX_3$ ($A = MA^+, FA^+, Cs^+$; $X = I, Br, Cl$), are now a very famous class of materials with applications in optoelectronic devices, such as solar cells, LEDs and lasers. The impressive interest aroused by LHPs is due to their remarkable optoelectronic properties (large absorption coefficients over the visible spectrum, long charge carrier diffusion lengths), combined with easy preparation, abundant constituent elements and broad compositional tunability [1]. The structural characterization and atomic-scale understanding of these materials is often challenging and the investigation of structure-properties relationship requires the combination of different methods. In these perspectives, Solid-State Nuclear Magnetic Resonance (SSNMR) stands out as characterization technique for LHPs for its ability to study ion dynamics, compositional variations and ion incorporation, chemical interactions, and degradation mechanisms [2]. In this contribution, recent studies on multiple-cation lead mixed-halide perovskite $Cs_{0.05}FA_{0.81}MA_{0.14}PbI_{2.55}Br_{0.45}$ [3], mono and multi layers 2D Ruddlesden-Popper (RP) phases containing butylammonium as spacer ($BA_2MA_{n-1}PbI_{n-3n+1}$ with $n=1-4$) [4], and $CsPbBr_3$ nanocrystals [5] will be presented and discussed, showing how multinuclear SSNMR (^{133}Cs , ^{207}Pb , ^{13}C , ^1H) can provide detailed information on structural and compositional disorder, organic cation dynamics and surface properties of nanocrystals. PRIN 2022 “**ISoTOPe - Combining Solid State NMR and CrysTal Engineering: a novel approach to probe Interfaces in 3D/2D Hybrid Metal Halide Perovskites**” funded by the European Union - Next Generation EU is acknowledged for financial support.

Keywords: Lead Halide Perovskites, Nuclear Magnetic Resonance, Structural and Dynamic Disorder, Material Science, Material Characterization

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ELECTRON-PHONON COUPLING IN TWO-DIMENSIONAL LEAD HALIDE PEROVSKITES

Tufan Ghosh^{a,*}, Vanga Ravali^a, Ram Ratan^b, E. Siva Subramaniam Iyer^b

^aDepartment of Chemistry, School of Advanced Sciences, VIT-AP University, Andhra Pradesh, 522237, India

^bSchool of Chemical and Materials Sciences, Indian Institute of Technology Goa, Ponda, Goa 403401, India

*Corresponding author: tufan.ghosh@vitap.ac.in

Abstract

Investigation of charge carrier dynamics, including the nature of coupling of the charge carriers with the lattice vibrational modes, is crucial to reveal the factors responsible for high photovoltaic efficiency in emerging two-dimensional (2D) lead halide perovskite (LHP). We use femtosecond transient absorption (TA) spectroscopy to uncover the ultrafast carrier relaxation dynamics in 2D lead halide perovskite thin films. Results from the TA measurements of the 2D (BA)₂(MA)_{n-1}PbI_{3n+1} (BA: n-butyl amine, MA: methylamine) perovskite films of varying inorganic layers, n = 1, 2, and 3 have been analyzed to estimate the hot carrier cooling time constants in each of these materials, the effect of the spacer cations on the cooling rates, and direct monitoring of electron-phonon coupling. Global analysis of the TA data from n = 1 perovskite films suggests that the hot carrier cooling to the band edge takes place with a time constant of 0.4 ps. Further, analysis of the TA data revealed weak periodic modulation of the transient absorption kinetic traces. These periodic modulations arise due to the modulation of the electronic susceptibility induced by coherently generated optical phonons in the materials. Fourier transform analysis of the residual modulations provides the frequency of the optic phonons in the range: 35 – 120 cm⁻¹, assigned to various modes of Pb-I inorganic framework. We believe that the detection of various low-frequency modes using femtosecond spectroscopy could provide useful insights into the electron-phonon coupling in 2D lead halide perovskite thin films.

Keywords: Two-dimensional perovskites, electron-phonon coupling, femtosecond spectroscopy

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INSIGHTS INTO THE DNA-BINDING MECHANISM OF CREN7: A RESILIENT PROTEIN FROM HARSH ENVIRONMENTS

Geethika K^a, Soumit S. Mandal^{a*},

Department of Chemistry, Indian Institute of Science Education and Research (IISER) Tirupati.

**Corresponding author: soumit.mandal@iisertirupati.ac.in*

Abstract

Crenarchaeal organisms thrive in extreme environments marked by high temperatures, salinity, and acidity. Their proteins exhibit remarkable structural stability, attributed to unique amino acid compositions. Cren7, a DNA-bending protein from these archaea, features a β -sheet structure with extended loops. UV melting assays show that DNA binding by Cren7 enhances thermal stability, preventing denaturation through both electrostatic and non-electrostatic interactions.

Fluorescence-based kinetic studies indicate that the solvent-exposed Trp26 (W26) is critical for stabilizing the Cren7–DNA complex under hypersaline conditions. Cren7 exhibits a preference for AT-rich DNA, binding with micromolar affinity. Circular dichroism (CD) spectroscopy reveals that DNA undergoes a cooperative structural change upon binding, while Cren7 retains its conformation.

Electrostatic interactions, primarily mediated by Lys31 (K31) and Lys27 (K27), play an essential role in DNA binding and complex stability. These roles are supported by biolayer interferometry and fluorescence anisotropy measurements.

The protein's hydrophobic core, stabilized by π -stacking interactions, also contributes to its structural robustness. Tyr58 (Y58) functions as a gatekeeper within this core. Alanine mutagenesis confirms that core residues are essential for the correct positioning of W26, reinforcing the importance of the hydrophobic core in DNA binding and bending. These findings emphasize the critical role of Cren7's structural features in maintaining complex stability and function under extremophilic conditions, contributing to the organism's adaptation.

Keywords: Crenarchaea, DNA binding, Electrostatic interaction, Hydrophobic interactions, Extremophiles

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NUCLEAR QUADRUPOLE RESONANCE FOR OBSERVING HALIDES AND THEIR PHOTOINDUCED SEGREGATION IN MIXED HALIDE PEROVSKITES

Silvia Borsacchi^{a,*}, Andrea Scarperi^b, Noemi Landi^a, Elisa Carignani^a, Marco Geppi^b

^a*Institute for the Chemistry of OrganoMetallic Compounds, National Research Council of Italy, CNR-ICCOM, via G. Moruzzi 1, 56124 Pisa, Italy*

^b*Department of Chemistry and Industrial Chemistry, University of Pisa, via G. Moruzzi 13, 56124 Pisa, Italy*

*Corresponding author: silvia.borsacchi@cnr.it

Abstract

Over the past decade, metal halide perovskites have emerged as one of the most promising classes of materials in photovoltaics due to their remarkable optoelectronic properties. In particular, mixed-halide perovskites of formula $\text{APb}(\text{X}_x\text{X}'_{1-x})_3$ (where A is typically methylammonium (MA), formamidinium (FA), or Cs^+ – and X is a halide anion) are known for their exceptional light-harvesting properties and for their tunable band gaps.¹ Despite their advantages, mixed-halide perovskites face stability issues. One of the main problems is that, under continuous illumination, perovskites of the type $\text{APb}(\text{Br}_x\text{I}_{1-x})_3$ undergo reversible phase segregation into I-rich and Br-rich domains (Hoke effect²), which compromises their performances. Understanding the structural modifications occurring during illumination, which rapidly revert in few minutes when illumination is removed, would significantly help to improve the stability and performance of perovskite-based devices. In this contribution we present one of the first cases of Nuclear Quadrupole Resonance spectroscopy³ applied to the observation of natural abundance ^{127}I and $^{79/81}\text{Br}$ isotopes in $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ compositions ranging from $x = 0.1$ to $x = 1$, proving how NQR can provide insights into halide distribution, particularly in highly mixed-halide systems. Moreover, we present the first ^{81}Br NQR investigation of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ perovskites under *in situ* illumination, providing the first experimental evidence of the effect of photoinduced halide segregation on NQR spectra, opening the way to the use of this spectroscopy for understanding photoinduced structural modifications occurring in metal halide perovskites.

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Keywords: perovskites, stability, structure, NQR, spectroscopy

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DESIGN AND SYNTHESIS OF PHOTOCONTROLLABLE PROBES FOR AMYOTROPHIC LATERAL SCLEROSIS STUDIES

Joseph Jen-Tse, Huang^{a*}

^a Institute of Chemistry, Academia Sinica, Taipei, 115, Taiwan

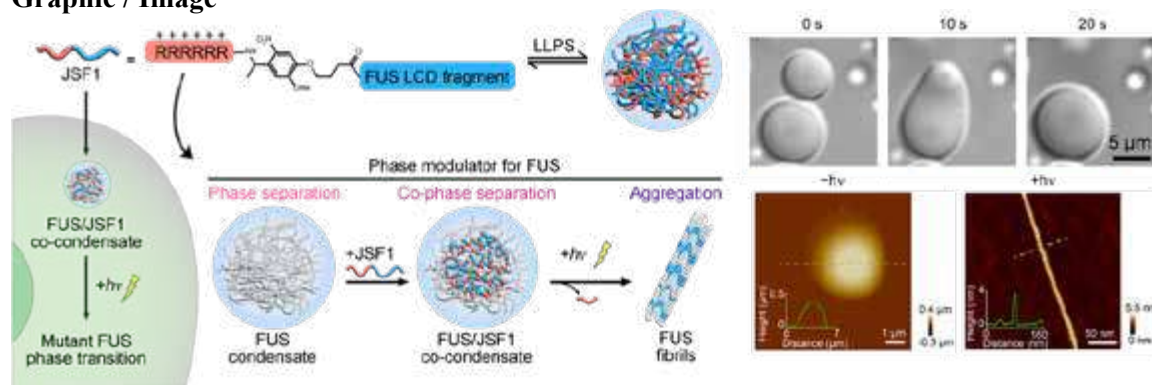
*Corresponding author: jthuang@gate.sinica.edu.tw

Abstract

TAR DNA-binding protein 43 (TDP-43) and fused in sarcoma (FUS) are nucleic acid-binding proteins involved in RNA processing and metabolism. Both proteins contain low complexity domains, which are critical for forming biological condensates. Misfolding of TDP-43 and FUS has been implicated in amyotrophic lateral sclerosis (ALS). In this context, we synthesized a series of photocontrollable TDP-43 probes that enable spatiotemporal control of amyloidogenic nanofibril formation in live cells, offering potential for early ALS diagnosis. Recently, studies have revealed a link between the phase transition of FUS condensates and their pathological maturation. As a result, modulating the phase behavior of these condensates has emerged as a key focus to understand their roles in disease. To this end, we developed a peptide-based phase modulator that forms droplets in the dark and transforms into amyloid-like fibrils upon light activation, confirmed through their distinct nanomechanical properties. This modulator enhances the condensation of recombinant FUS protein and induces fibrilization when exposed to light. We further applied this tool to regulate the biophysical states of FUS condensates in live cells, exploring the connection between FUS phase transitions and proteinopathy. These findings provide insights into how protein phase transitions influence cellular function and dysfunction.

Keywords: Photocontrollable peptide, TDP-43, FUS, phase separation, ALS

Graphic / Image



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ULTRAFAST DYNAMICS OF DAMAGED DNA REPAIR BY A DUAL FUNCTION CRYPTOCHROME

Dongping Zhong*

Center for Ultrafast Science and Technology, School of Chemistry and Chemical Engineering, Zhangjiang Institute for Advanced Study, Shanghai Jiao Tong University, Shanghai, China

**Corresponding author: dongping@sjtu.edu.cn*

Abstract

Photolyase and cryptochrome belong to a group of structurally similar flavoproteins but with two distinct functions of DNA repair as a photoenzyme and signal transduction as a photoreceptor, respectively, under blue-light illumination. Here, we studied a recently discovered bifunctional *Chlamydomonas reinhardtii* cryptochrome (CraCRY) with focus on its repair of UV-induced pyrimidine-pyrimidine (6-4) photoproduct (6-4PP). We used femtosecond spectroscopy and site-directed mutagenesis to map out the critical elementary steps by following the dynamics of initial reactants, various intermediates and final products. We observed initial direct ultrafast electron tunneling from the hydroquinone flavin cofactor to 6-4PP in 300 ps through an intervening adenine as a mediator, minimizing the electron bifurcation of a two-step hopping pathway bridged also by the adenine as an intermediate. The subsequent proton transfer from the neighboring histidine to anionic 6-4PP in 2 ns is critical and competes with the futile back electron transfer in 151 ps. Mutations of either of two histidines in the active site nearly abolish repair, indicating their essential role on repair reactivity and structural integrity. These results elucidate the electron-coupled proton transfer (ECPT) mechanism and the repair photocycle of this bifunctional cryptochrome at the molecular level, further supporting that the hydroquinone flavin is the active state *in vivo* for dual functions or one of the two functions is excessive.

Keywords: 6-4 repair, photocycle, enzymatic reaction, electron bifurcation, proton transfer

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MOLECULAR ORIGIN AND QUENCHING MECHANISM OF PHOTOLUMINESCENT CARBON QUANTUM DOTS FROM AMMONIUM CITRATE

Wan Ryan Asri^{1*}, Asem Alenaizan¹, Mohammad N. Siddiqui¹, and Almaz Jalilov^{2,3}

¹ Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

² Department of Biology, Chemistry and Environmental Sciences, American University of Sharjah, P.O. Box 26666, Sharjah, United Arab Emirates

³ Materials Research Center, American University of Sharjah, P.O. Box 26666, Sharjah, United Arab Emirates

*Corresponding author: g202213620@kfupm.edu.sa

Abstract

Carbon quantum dots (CQDs) possess tunable photoluminescence (PL), excellent biocompatibility, and low toxicity, making them highly promising for various applications. Unlike conventional semiconductor quantum dots (SQDs), whose PL centers arise from well-defined bandgap-related electronic transitions, CQDs exhibit diverse and interdependent PL centers including carbon-core, molecular, and carbon states. These complex emissive origins, coupled with the structural inherent of CQDs, present challenges in fully understanding and optimizing their PL properties for broader applications. Herein, the PL features of two CQDs synthesized from di- and tri-ammonium citrate via cost-effective pyrolysis method at 150 °C and 40 h were systematically investigated. Through concentration-dependent analyses, it was found that at lower concentration, both CQDs possessed nanoparticle-like behavior, with aggregation-induced emissions leading to the enhancement of PL emission. Upon elevating concentration, aggregation-induced quenching of PL emission became prominent. Time-resolved PL spectroscopy revealed that the primary emissive centers of CQDs originate from edge-functionalized groups (long component) and aromatic π -conjugated domains (short component), corresponding to surface and carbon-core states, respectively. Additionally, quenching studies using electron donors and acceptors provided insights into the dynamic PL mechanism of CQDs. These findings contribute to a deeper understanding of CQDs' PL behavior, paving the way for their effective application in diverse fields.

Keywords: ammonium citrate, carbon quantum dots, photoluminescence, quenching studies.

INTERFACIAL ACCUMULATION OF POLYMERS IN EMULSIFIED AQUEOUS MULTIPHASE SYSTEMS

Daniel Pliego Sosa^a, Jan van Esch^{a*}

^a*Delft University of Technology (TU Delft)*

^{*}*Corresponding author: j.h.vanesch@tudelft.nl*

Abstract

The phase separation of aqueous polymer solutions due to thermodynamic processes is relatively well understood and described by several theories.¹ In aqueous multiphase systems (AMPS), polymer solutions typically separate into macroscopic phases;² however, when emulsified, these polymer phases can form microscopic domains with either a 3D-bulk or 2D-interfacial spatial organization.³ Despite its potential significance, the interfacial accumulation of polymers in emulsified AMPS remains largely unexplored, with limited literature and an incomplete understanding of its underlying mechanisms.

In this study, we found that introducing small amounts of a third polymer into emulsified aqueous two-phase systems led to its preferential accumulation at the interface between the two main phases. This behavior does not appear to be universal but rather depends on specific system parameters, including the polymer type, molecular weight, and concentration of the third polymer. We investigated the role of interfacial free energy minimization as a driving force for this accumulation and proposed a refined mechanism to explain the phenomenon.

Our findings provide new insights into the mechanisms governing interfacial polymer accumulation in emulsified AMPS. While further research is needed for a more comprehensive understanding, this work opens new possibilities for microstructuring aqueous polymer solutions both at the interface and in the bulk. These insights could lead to advancements in fields that require precise spatial organization of polymers, such as drug delivery, biocatalysis, and biosensors.

Keywords: Aqueous multiphase systems, polymer phase separation, interfacial accumulation, water-in-water emulsions.

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STUDYING MULTIPHASE REACTIONS IN MICRODROPLETS VIA SINGLE PARTICLE SPECTROSCOPIC PLATFORM

Yuan-Pin Chang^{a*}

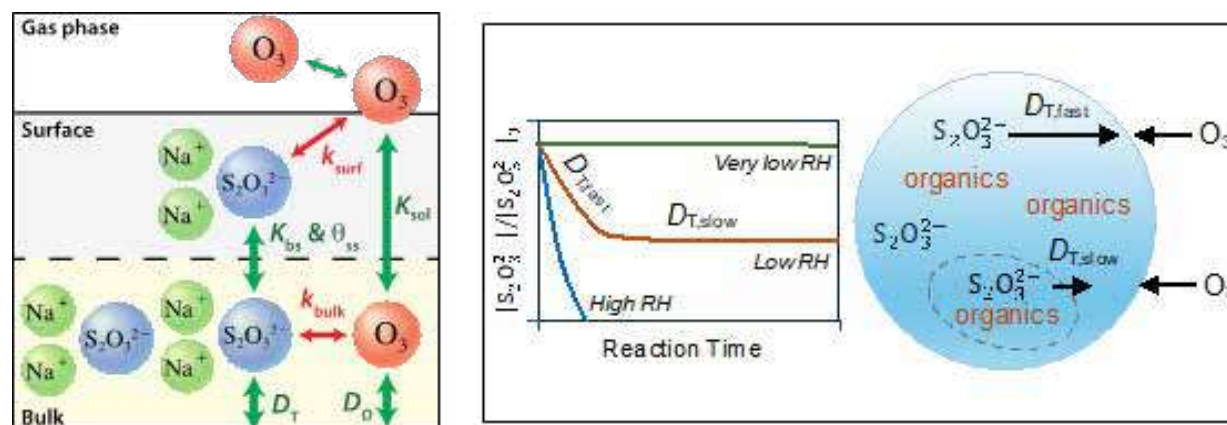
^a Department of Chemistry, National Sun Yat-sen University, Taiwan.

*Corresponding author: ypchang@mail.nsysu.edu.tw

Abstract

This presentation will summarize our recent works of exploiting aerosol optical tweezers coupled with Raman spectroscopy to investigate multiphase reactions in optically trapped single microdroplets, including the interfacial oxidation reaction of aqueous thiosulfate and gaseous ozone and the conversion of gaseous formaldehyde to aqueous methanediol.¹⁻² The aim is to elucidate the roles of interface and bulk reactions in aerosol chemistry and the complicate interplays between physicochemical properties and multiphase chemistry of atmospheric aerosol. The time-resolved Raman spectra of optically trapped single microdroplets allows for retrieving various physicochemical properties of each optically trapped microdroplet, such as droplet radius, refractive index, solute concentrations, pH, ionic strength, diffusivity ... etc. Furthermore, a multi-layer kinetic model dedicated to aerosol chemistry is used to simulate multiphase reactions on the aerosol surface and in the bulk phase under different conditions, allowing for clarifying the roles of surface and bulk reactions in aerosol reaction kinetics.³ These results demonstrates that the application of such single particle spectroscopic platform can be a versatile tool to elucidate the multiphase nature of aerosol reaction kinetics.

Keywords: Aerosol, Raman spectroscopy, Reaction kinetics, Atmospheric chemistry, Multiphase chemistry



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COMPUTATIONAL SCREENING OF NOVEL INHIBITORS FROM AN IN-HOUSE LIBRARY TARGETING THE LIGAND BINDING DOMAIN OF HUMAN ANDROGEN RECEPTOR

Bodee Nutho^{a*}, Phakkhathorn Tadasee^a, Tanatorn Khotavivattana^b

^aDepartment of Pharmacology, Faculty of Science, Mahidol University, Thailand

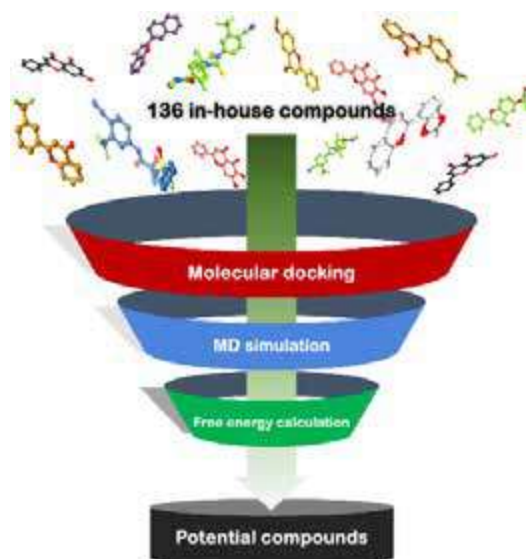
^bDepartment of Chemistry, Faculty of Science, Chulalongkorn University, Thailand

*Corresponding author: bodee.nut@mahidol.ac.th

Abstract

Abnormal androgen receptor (AR) expression is the most common cause of prostate cancer (PCa) in men. Androgen deprivation therapy plays a pivotal role in suppressing AR expression. However, the use of these drugs is limited by their side effects and the emergence of drug resistance. Hence, there is a critical need to discover new drug therapies for PCa patients. Non-steroidal compounds, known for their diverse biological activities, are particularly promising in anti-PCa therapy. In this study, we pre-screened a series of non-steroidal compounds from our in-house library for their anti-PCa potential using *in silico* methods. We initially assessed the binding affinity of these compounds to AR ligand binding domain (LBD) through molecular docking. The docking results revealed that compounds **18ad**, **18ai** and **18aj** exhibited superior binding affinity against the targeted protein compared to both the positive controls and other compounds. Moreover, molecular dynamics (MD) simulations showed that these complexes were relatively stable, highlighting key residues for ligand binding such as L704, G708, M742, M745, V746, M749, F764, L873, T877 and M895. Therefore, our findings from these computational approaches signify an important step toward discovering novel compounds targeting the LBD of AR for PCa therapy.

Keywords: prostate cancer, androgen receptor, molecular docking, molecular dynamics simulation



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HOST-GUEST COMPLEXATION OF DAPIVIRINE AND CUCURBIT[n]URIL: INSIGHT FROM MOLECULAR DYNAMICS SIMULATION

Nadtanet Nunthaboot*, Jirasak Thippichai, Chananya Rajchakom, Thitiya Boonma

*Multidisciplinary Research Unit of Pure and Applied Chemistry and Supramolecular Chemistry Research Unit,
Department of Chemistry and Center of Excellence for Innovation in Chemistry (PERCH-CIC), Faculty of Science,
Mahasarakham University, Maha Sarakham 44150, Thailand*

**Corresponding author: nadtanet.n@msu.ac.th*

Abstract

This study aims to investigate the influence of cucurbit[n]uril (CB[n]), where $n = 6, 7, 8$, and 10 , specifically cucurbit[6]uril, cucurbit[7]uril, cucurbit[8]uril, and cucurbit[10]uril, on the encapsulation and binding of dapivirine, an antiviral drug used for HIV prevention. The study employs molecular docking and molecular dynamics (MD) simulation to analyse host-guest interactions. The 1:1 complexation study reveals that the binding mode of dapivirine within the host cavity is dependent on the cavity size. Cucurbit[6]uril accommodates dapivirine with its benzonitrile moiety oriented inside the cavity, while cucurbit[7]uril and cucurbit[8]uril can encapsulate dapivirine with either benzonitrile or trimethylanilino facing inward. In contrast, cucurbit[10]uril, with its larger cavity, fully encapsulates the dapivirine molecule. The binding energy calculations indicate that cucurbit[10]uril exhibits the most stable binding interaction compared to cucurbit[8]uril, cucurbit[7]uril, and cucurbit[6]uril, respectively. These findings highlight the crucial role of cavity size and host chemical properties in guest accommodation and complex stability.

Keywords: Cucurbit[n]uril, Dapivirine, Docking, Inclusion, HIV inhibitor

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REACTION DYNAMIC IN SOLUTION PROBED BY FEMTOSECOND INFRARED SPECTROSCOPY

Seongchul Park^a, Hojeong Yoon^a, Manho Lim^a

^a*Pusan National University.*

**Corresponding author: mhl@pusan.ac.kr*

Abstract

Although chemical reaction dynamics of isolated molecules has been extensively explored and understood, that in liquid phase is much less comprehended due to the complication of solvent-solute interaction. Recent advances in ultrafast spectroscopic techniques make it possible to obtain a detailed information on the reaction dynamics in liquids. In particular, time-resolved infrared (IR) spectroscopy can probe transient molecular structures involved in chemical reaction pathways, providing critical information needed in solving the mechanisms of chemical reactions. Here, photodissociation dynamics of $\text{CF}_2\text{BrCF}_2\text{I}$ in CCl_4 solution was investigated by probing the C–F stretching mode from 300 fs to 10 μs after excitation at 267 nm using femtosecond time-resolved infrared spectroscopy. We were able to compose complete photolysis dynamics of $\text{CF}_2\text{BrCF}_2\text{I}$ in solution including the fate of all the produced intermediates. In addition, we found that the CF_2BrCF_2 radical in CCl_4 solution rotationally isomerizes with a time constant of 47 ± 5 ps at 280 ± 2 K. From this value and the rotational barrier heights of related compounds, we determined rotational isomerization time of carbon–carbon single bonds in ethyl radical and ethyl derivatives in room-temperature solution

Keywords: reactions in solutions, rotational isomerization, photodissociation, time-resolved spectroscopy

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PHOTOPHYSICAL PROPERTIES OF 3,3'-DIETHYLTHIACARBOCYANINE IODIDE (Cy3) FLUORESCENT MOLECULAR ROTOR IN DEEP EUTETIC SOLVENTS AND ORGANIC MOLECULAR SOLVENTS

Mohd Azizi Nawawi^{a,*}, Putri Nurfarrah Syofea Rosllan^a, Norhafizah Jaafar^a,
Muhammad Arif Danial Zazuli^a

^a*School of Chemistry and Environment, Faculty of Applied Sciences, Universiti Teknologi MARA 40450 Shah Alam, Selangor Malaysia*

^{*}*Corresponding author: azizi_nawawi@uitm.edu.my*

Abstract

Fluorescent molecular rotors are a class of fluorescent dyes whose emission properties are sensitive to the viscosity or microenvironment of their surroundings. These molecules contain rotatable chemical bonds that can undergo intramolecular twisting upon light excitation. In low-viscosity environments, the rotation leads to non-radiative energy loss and weak fluorescence signal. In contrast, restricted rotation in high-viscosity or crowded environments results in strong fluorescence signal. While viscosity sensitivity is the defining feature of molecular rotors, some are also polarity-sensitive, especially if they have features like intramolecular charge transfer (ICT). This unique behaviour makes molecular rotors valuable tools in biological imaging, materials science, and viscosity sensing at the micro- or nanoscale. In this work, photophysical of a fluorescent molecular rotor, 3,3'-diethylthiacarbocyanine (Cy3) were measured in a series of deep eutectic solvents (DES) and organic molecular solvents (OMS) of different viscosity and polarity. The Förster-Hoffmann equation was used to describe the relationship between the fluorescence emission intensity of Cy3 and the viscosity of medium. The fluorescence emission intensity of Cy3 was observed to increase linearly with increasing viscosity of both types of solvent with correlation coefficients (R^2) of 0.8029 for DES and $R^2 = 0.965$ and $R^2 = 0.7691$ for polar and non-polar OMS, respectively. These linear relationships show that fluorescence signal of Cy3 is highly sensitive to changes in viscosity of solvent with a slight sensitivity towards solvent polarity. Therefore, Cy3 can be a potential chemical probe for measuring the local viscosity especially when measurement of viscosity by the traditional equipment or technique is unfeasible due to some constraint in terms of amount of sample or complexity of system. Additionally, the results may provide deeper insights into solute-solvent interactions, helping to understand how molecules behave in various environments, such as ionic and non-ionic solvents.

Keywords: viscosity, polarity, deep eutectic solvent, fluorescent molecular rotor, Förster-Hoffmann equation

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STOICHIOMETRIC AND CATALYTIC REACTIONS WITH N-HETEROCYCLIC CARBENE PINCER LIGANDS

Pierre Braunstein^{a*}

^aUniversity of Strasbourg – CNRS, Institute of Chemistry, 67081 Strasbourg (France)

*Corresponding author: braunstein@unistra.fr

Abstract

The reactivity of organometallic complexes and of homogeneous metal-based catalysts largely depends on the control of the metal coordination sphere exerted by the ligands. This accounts for the growing interest in multifunctional ligands, particularly with chemically different donor functionalities and / or constrained geometries.¹ *N*-Heterocyclic carbene (NHC) ligands (Figure 1), bearing additional donor groups with significantly different stereoelectronic properties, are ideal candidates for studying the chemoselectivity of their coordination to metal centres and its impact on the reactivity of the corresponding metal complexes.² Furthermore, NHC donors can be introduced in pincer-type structures (Figure 2),³ and unexpected reactivity of C–H and C–P bonds have been observed with Ni and Pd complexes bearing N^{imine}C^{NHC}N^{imine} or PC^{NHC}P pincer ligands.^{4,5}

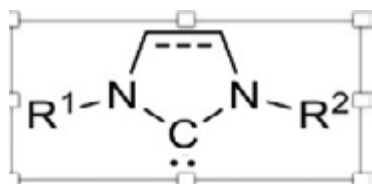


Figure 1. Typical structure of a *N*-Heterocyclic Carbene (NHC) Ligand

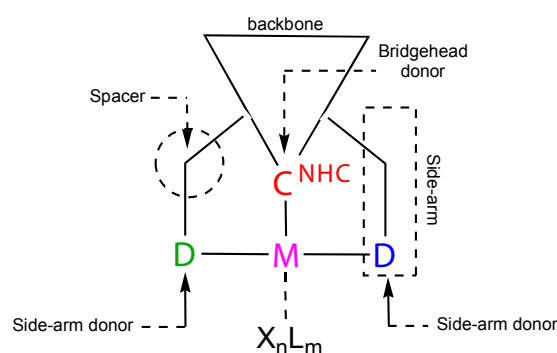


Figure 2. Generic structure of a pincer complex with a NHC donor in the bridgehead position.³

Keywords: Organometallic Reactivity, Functional Ligands, *N*-Heterocyclic Carbenes, Transition Metal Pincer Complexes, Bond Activation

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CONTROL OF EXCITED STATES, NANOSTRUCTURES AND FUNCTIONS THROUGH MOLECULAR DESIGN AND SUPRAMOLECULAR ASSEMBLY

Vivian Wing-Wah YAM^{a,*}

^a *Institute of Molecular Functional Materials and Department of Chemistry,
The University of Hong Kong, Pokfulam Road, Hong Kong, PR China*

**Corresponding author: wwyam@hku.hk*

Abstract

Works in our laboratory have shown that novel classes of light-absorbing and luminescent metal-containing molecular materials could be assembled through the use of various metal-ligand chromophoric motifs. In this presentation, various design and synthetic strategies for new classes of chromophoric and luminescent metal complexes will be described. A number of these metal-ligand chromophoric complexes have been shown to display rich luminescence and photofunctional behavior.¹ The chromophoric and luminescence behavior have been studied. Correlations of the chromophoric and luminescence behavior with the electronic and structural effects of the metal complexes have been made to elucidate their spectroscopic origins. Some of these simple discrete metal complexes are found to undergo supramolecular self-assembly¹⁻⁵ or co-assembly^{1,6,7} with block copolymers to give a variety of nanostructures and morphologies with different colors and emission properties. Subtle changes in the microenvironment, conformations and nanostructured morphologies have led to drastic changes in both the electronic absorption and emission properties of these hierarchical supramolecular assemblies.¹⁻⁷ Explorations into the underlying factors that determine their spectroscopic properties and morphologies as well as their assembly processes have provided new insights into the understanding of their photophysics, structure-property-function relationships, and the interplay of the various intermolecular forces and interactions for the directed assembly of metal-containing supramolecular assemblies and soft materials.¹⁻⁷ Manipulation of the electronic effects, molecular conformation, orientation and assembly has led to the control of the excited states in novel molecular materials and supramolecular assemblies.^{1,3-7} The exploration into the potential applications and functions of these light-emitting discrete metal complexes, supramolecular assemblies and polymers will also be described.

Keywords: Supramolecular Assembly; Luminescence; Metal-Containing Functional Materials

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OPTIMISING PYROCHLORE STRUCTURED FUNCTIONAL CERAMICS: PROCESSING CONTROL, PHASE EQUILIBRIA, MICROSTRUCTURAL AND ELECTRICAL PROPERTIES

Kar Ban Tan

Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, UPM 43400, Serdang, Selangor
Corresponding author: tankarban@upm.edu.my

Abstract

Precise control of ceramic processing is paramount for optimising product quality, reliability and performance. This control significantly influences the microstructure and resultant mechanical, thermal, electrical and optical properties of the ceramic materials. Stringent process control not only minimises production costs and ensures environmentally benign manufacturing but also fosters innovation in materials tailored to specific applications, ranging from electronics to structural components. This presentation details the synthesis and characterisation of bismuth-containing pyrochlore systems, focusing on their phase equilibria, crystallo-chemical and dielectric properties. Technical data collected by both spectroscopic and microscopic techniques were utilised to correlate composition, structure and properties of these functional ceramics. Crucially, rigorous optimisation and processing were essential for achieving single-phase pyrochlore synthesis, maintaining thermal equilibrium and preventing bismuth volatilisation. This required exhaustive sample preparation for detailed phase evolution and equilibrium studies prior to construction of ternary phase diagrams, employing comprehensive quantitative and qualitative powder XRD analyses complemented by the disappearing phase method. The phase-pure pyrochlore subsolidus regions, phase compatibilities and phase assemblages between various phases were successfully identified. Consequently, doping mechanisms, utilising different compositional variables, were employed to describe the subsolidus solution areas, ensuring the overall charge electroneutrality of the systems. Furthermore, impedance data, superimposed on the pyrochlore subsolidus solution regions, illustrate the compositional influence on their dielectric properties. In conclusion, these findings provide further insights and broader understanding of various pyrochlore systems and their application in the development of high-performance ceramic capacitors.

Keywords: ceramics, pyrochlores, optimisation, phase equilibria, impedance

PEROVSKITE BARIUM TANTALUM OXYNITRIDE: FROM MATERIALS SYNTHESIS TO SOLAR WATER SPLITTING

Mirabbos Hojamberdiev*

Mads Clausen Institute, University of Southern Denmark, Alsion 2, 6400 Sønderborg, Denmark

*Corresponding author: mirabbos@mci.sdu.dk

Abstract

Although hydrogen is a zero-emission energy carrier, its current global production still heavily relies on fossil fuels. Current momentum on renewable energy and environmental remediation is unprecedented because of fast climate change. We all know the world is hurrying to achieve the United Nations Sustainable Development Goals (SDGs) by 2030. One of the important SDGs is Goal 7: Affordable and Clean Energy. As a replica of natural photosynthesis, a semiconductor-based artificial photosynthetic system is regarded as one of the most economically viable, highly efficient, and environmentally benign chemical processes to generate green hydrogen energy from solar water splitting. However, to harness solar energy efficiently, it is necessary to enhance the visible-light-driven photocatalytic performance of the existing materials and to discover novel visible-light-active materials. Mixed-anion compounds offer new opportunities in this regard [1]. As a 600 nm-class photocatalyst, BaTaO₂N has received particular attention due to its small bandgap ($E_g = 1.8$ eV), suitable band edge positions for visible-light-induced water splitting, chemical stability, and nontoxicity [2,3]. BaTaO₂N is routinely synthesized by a two-step method: (i) the synthesis of a corresponding oxide precursor and (ii) its high-temperature nitridation under an NH₃ atmosphere for a prolonged period. However, this two-step method leads to the formation of various defects that negatively affect the water-splitting performance. Therefore, we have applied an NH₃-assisted direct flux growth approach to reduce the defect density of BaTaO₂N, engineered the bandgap by cation doping, and explored the effects of the altered morphology, size, and porosity on the visible-light-induced water oxidation activity and photoelectrochemical performance of BaTaO₂N. The findings revealed that the photocatalytic activity and photoelectrochemical performance of BaTaO₂N were significantly influenced by particle morphology, size, porosity, dopant type, and doping amount. Particularly, the BaTaO₂N crystal structures obtained by nitridation of the oxide precursor without KCl flux exhibited a higher surface area and high anodic photocurrents compared to the BaTaO₂N crystal structures obtained by nitridation of the oxide precursor with KCl flux due to the high number of dangling bonds acting as nucleation centers for the highly dispersed CoO_x cocatalyst nanoparticles.

Keywords: Oxynitrides, BaTaO₂N, Water splitting, Green hydrogen, Photocatalysis

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VISIBLE-EMITTING RARE EARTH COMPLEXES FOR SENSING AND SOLAR ENERGY CONVERSION

Lidia Armelao^{a,b}

^aDepartment of Chemical Sciences, University of Padova, Via Marzolo 1, 35131 Padova, Italy

^bDepartment of Chemical Sciences and Materials Technology, National Research Council (CNR),
Piazzale A. Moro 7, 00185 Roma, Italy

*Corresponding author: lidia.armelao@unipd.it

Abstract

Complexes of rare-earth ions (RE^{3+}) represent a vast source and a promising approach for the development of luminescent functional materials. To fully exploit their properties, it is necessary to develop versatile synthetic protocols, investigate in detail the correlations between different molecular fragments, emission, and functional properties. Furthermore, it is crucial to develop synthetic approaches that enable the processability of luminescent complexes to achieve materials and devices that maintain or even enhance the functional properties. In this context, we have focused on β -diketonate complexes as a platform for our research. They are a well-known and extensively studied class of complexes commonly used to sensitize the luminescence of RE^{3+} ions via the so-called *antenna effect*. The spectroscopic properties of β -diketonates can be modulated by varying the nature of the R,R' substituent groups and the ancillary ligands that complete the coordination sphere of the cation.¹ Moreover, through appropriate functionalization, it is possible to modulate the number, type, and relative position of the binding sites in the ligands, thus controlling the number and spatial organization of the RE^{3+} cations in the complex.^{2,3} This modulation allows obtaining monometallic complexes, dimers, oligomers, and even extended structures such as coordination polymers or MOFs. In addition to multinuclear complexes containing only -4f ions, a careful choice of the binding sites on the ancillary ligands allows the preparation of heterometallic systems containing -4f and -d or -p block cations,⁴ thus expanding the possibilities for optimizing and improving the functional properties. Following this synthesis strategy, we used luminescent complexes of Eu^{3+} and Tb^{3+} to develop molecular thermometers and for the sensing of small chiral molecules. By integrating the complexes into polymeric matrices we obtained highly luminescent and transparent materials employed for the development of solar energy conversion devices.^{5,6}

Keywords: Rare earth luminescence, molecular thermometers, luminescent solar concentrators

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PHOSPHINE-STABILIZED DICARBON AND ITS CHEMISTRY

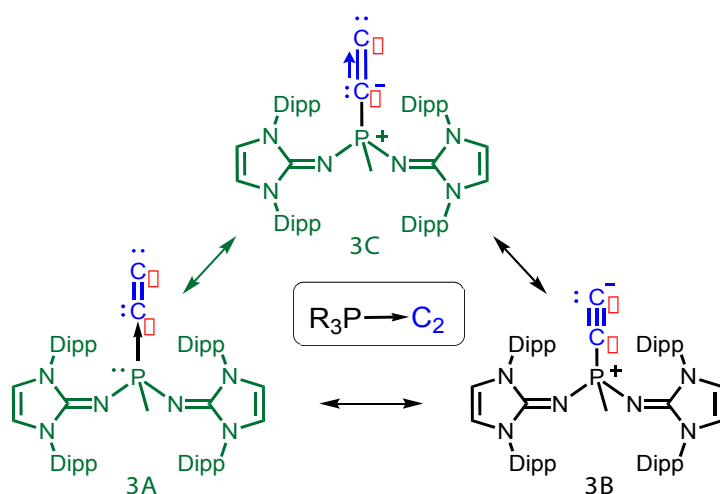
Tiow-Gan Ong^{a,*}

Institute of Chemistry, Academia Sinica, Taipei, 115201, Taiwan, Republic of China^a.

**Corresponding author: tgong@gate.sinica.edu.tw*

Abstract

Elusive diatomic C_2 has been prepared and structurally characterized as mono-ligated complex $L \rightarrow C_2$ using a bulky bis(imidazolidin-2-iminato)methylphosphino ligand $L = (NHC^R=N)_2(CH_3)P$. The compound is stable in solution at ambient temperature and can even be isolated in the solid state. The reactivity has been investigated with a variety of reactions, suggesting the two lone-pairs residing between two adjacent carbons (C_β and C_α).^[1] The nature of the $L \rightarrow C_2$ bond was also studied with quantum chemical methods to understand the nature of bonding. The successful isolation of a stable complex of C_2 ligated by a phosphine offers application in the transition metal coordination chemistry and catalysis.^[2]



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PLASMONIC AND MAGNETIC NANOPARTICLES FOR BIOMEDICAL APPLICATIONS

Nguyen Thi Kim Thanh MAE FRSC FInstP FRSB FAPS FIMMM

Biophysics Group, Department of Physics and Astronomy, University College London, and UCL Healthcare

Biomagnetics and Nanomaterials Laboratory

21 Albemarle Street, London W1S 4BS, London, UK

**Corresponding author: ntk.thanh@ucl.ac.uk*

Abstract

The development of new chemical methods for the next generation of nanoparticles with very high magnetic moment, fine tuning Au nanorods and novel hybrid and multifunctional nanostructure is presented. Detailed mechanistic studies of their formation by sophisticated and advanced analysis of the nanostructure allows tuning of the physical properties at the nanoscale; these can subsequently be exploited for diagnosis and treatment of various diseases. The studies are conducted to provide insight for future material design approaches. It will also help to identify the critical process parameters that can be manipulated in order to obtain the suitable physical properties for the intended applications.

Keywords: Nanoparticles, magnetic hyperthermia, MRI contrast agent, infectious diseases and cancers

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DESIGNING TRANSITION METAL-BASED NANOSTRUCTURES FOR SUSTAINABLE PHOTO-CATALYSIS

Kalyanjyoti Deori*, Priyanka Gogoi, Soniya Agarwal, Ramani Hazarika

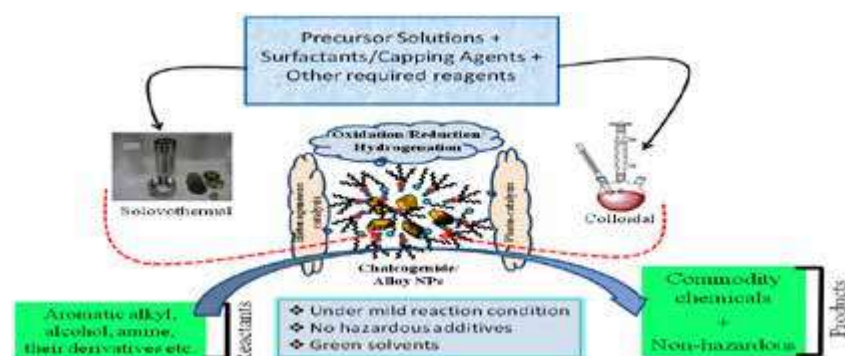
^aKD's 'NAME (NanoMat&Energy) Lab, Department of Chemistry, Dibrugarh University, Dibrugarh, Assam, India 786004.

*Corresponding author: kalchemdu@gmail.com; kalchemdu@dibru.ac.in

Abstract

Out of various transition metal-based nanostructures binary metal chalcogenides and alloy nanoparticles represent a promising yet underexplored class of materials for heterogeneous catalysis in industrially significant organic transformations. While these materials are predominantly recognized for their exceptional optical, electronic, and magnetic properties—arising from their semiconducting behavior, structural stability, and synergistic effects—they have been primarily utilized in applications such as optics, electronics, magnetism, fuel cells, and antibacterial activity. However, recent studies have begun to highlight their unique catalytic potential in organic reactions, opening up tremendous opportunities for future research in this domain. In this work, we present a straightforward hydrothermal/solvothermal approach, complemented by a surfactant-assisted colloidal strategy, to synthesize 3d transition metal-based binary chalcogenide and alloy nanoparticles with diverse and tunable morphologies. By carefully controlling reaction parameters, we achieved precise morphological tailoring, enabling the development of efficient heterogeneous multifunctional photocatalysts for a range of industrially significant organic reactions. The structural and morphological properties of the synthesized nanoparticles were thoroughly characterized using techniques such as XRD, HRTEM etc. These novel nanostructured chalcogenides and alloys demonstrated remarkable catalytic activity, excellent conversion efficiency, and superior recyclability in various organic transformations. Their exceptional performance highlights their potential as model systems for sustainable catalysis research, paving the way for their application in future catalytic technologies.

Keywords: Photocatalysis, chalcogenides, alloys, nanostructured catalyst, multifunctional



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UNLOCKING COBALT OXIDE'S POTENTIAL: ADVANCING PHOTOELECTROCHEMICAL HYDROGEN PRODUCTION BEYOND CONVENTIONAL MATERIALS

Siti Nurul Falaein Moridon^a, Khuzaimah Arifin^{a,b}, Mohd Ikhmal Salehmin^{a,c}, Mohamad Azuwa Mohamed^{a,d}, Lorna Jeffery Minggu^a, Mohammad B. Kassim^{a,d,*}

^a*Fuel Cell Institute, Universiti Kebangsaan Malaysia, 43600, UKM Bangi, Selangor, Malaysia*

^b*Research Center for Advanced Materials, National Research and Innovation Agency (BRIN), 224 Building, Puspiptek Area, South Tangerang, 15314, Indonesia*

^c*Seksyen Pembangunan Teknologi dan Produk, Pusat Nanoteknologi Kebangsaan (PNK), Kementerian Sains, Teknologi, dan Inovasi (MOSTI), Aras 4, Blok C7, Kompleks C, Pusat Pentadbiran Kerajaan Persekutuan, 62662 Putrajaya, Malaysia*

^d*Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600, UKM Bangi, Selangor, Malaysia*

**Corresponding author: mb_kassim@ukm.edu.my*

Abstract

The global shift towards sustainable energy has heightened the need for efficient photoelectrochemical (PEC) systems to produce clean hydrogen fuel. While titanium dioxide (TiO₂) has been widely used, its limitations in efficiency and stability necessitate the search for superior alternatives. Cobalt oxide (Co_xO_y) has recently emerged as a promising candidate due to its excellent catalytic properties and favorable electronic structure for PEC water splitting. This study aims to investigate the PEC performance of cobalt oxide, focusing on the Co₃O₄ phase, and compare its hydrogen production efficiency and stability against TiO₂, a conventional photocatalyst. Cobalt oxide was synthesized using a hydrothermal method, followed by annealing at varying temperatures to optimize phase formation. The resulting materials were characterized to confirm the formation of the Co₃O₄ phase. The PEC activity was evaluated through photocurrent density measurements (vs. Ag/AgCl) and hydrogen evolution rates under simulated solar illumination. The optimized Co₃O₄ phase demonstrated a photocurrent density of 1.15 mA cm⁻² at -0.4 V vs. Ag/AgCl, nearly twice the values typically reported for TiO₂-based systems. In hydrogen evolution tests, Co₃O₄ achieved a production rate of 272.6 μmol h⁻¹g⁻¹ over 8 hours and exhibited stable performance for over 12 hours, outperforming TiO₂ in both efficiency and durability. The findings establish cobalt oxide, particularly the Co₃O₄ phase, as a high-performing, stable, and scalable alternative to TiO₂ for PEC hydrogen production. This study highlights cobalt oxide's potential to contribute to the advancement of efficient and sustainable hydrogen generation technologies.

Keywords: Hydrogen, cobalt oxide, titanium dioxide, photocatalyst, PEC

DESIGN, SYNTHESIS, AND PROPERTY OPTIMIZATION OF INORGANIC FUNCTIONAL MATERIALS: FROM ATOMIC STRUCTURE TO MACROSCOPIC PERFORMANCE

Ling Chen^{a, b*}

^aCollege of Chemistry, Beijing Normal University, Beijing 100875, People's Republic of China

^bState Key Laboratory of New Textile Materials and Advanced Processing, Wuhan Textile University, Wuhan 430200, People's Republic of China

*Corresponding author: chenl@bnu.edu.cn; chenling@wtu.edu.cn

Abstract

Our research presents innovative strategies to enhance material performance through crystal engineering and structural design. Special emphasis is placed on understanding how atomic-level structural modifications influence macroscopic material properties, including second-order nonlinear optical properties or thermoelectric properties. We demonstrate how anisotropic structural units and π confinement effects can optimize deep-UV optical properties.^[1-3] For thermoelectric materials, we reveal how valence band convergence and two-dimensional coordination geometry allowing 2D phonon scattering enable breakthrough thermoelectric performance.^[4, 5]

We establishing design principles linking chemical bonding anisotropy to NLO responses, developing crystal engineering approaches to enhance optical nonlinearity and balancing property trade-offs, and demonstrating anisotropic local coordination for ultralow thermal conductivity.

Keywords: Solid state chemistry, Second harmonic generation, thermal conductivity

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NHC AND PHOSPHINOUS ACID PALLADIUM PRECATALYSTS: EFFICIENT CATALYSIS IN KUMADA AND SEVERAL CROSS-COUPLING REACTIONS

Yu-Chang Chang^{a*}

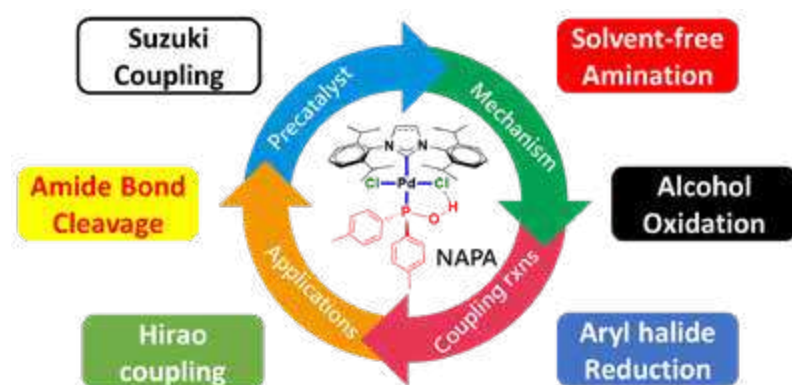
^a Department of Applied Chemistry, Providence University, 200, Sec. 7, Taiwan Boulevard, Shalu Dist., Taichung City 43301 Taiwan

*Corresponding author: vickchang@pu.edu.tw

Abstract

A series of highly effective NHC and phosphinous acid-based palladium precatalysts (NAPA), (NHC-PdCl₂-PAR₂(OH)), and their efficiency in catalyzing Kumada-Tamano-Corriu (KTC) and several cross-coupling reactions are reported. Taking KTC couplings, for example, the NAPA-catalyzed reactions could reach high yields at 50 °C in 3 hours. Higher substituted biaryl products obtained good results by raising the temperature to 80 °C for 3 hours. A dropwise addition method was employed to address functional group tolerance issues in reactions of Grignard reagents with aryl chlorides in KTC couplings. Upon deprotonation of the ligated PAR₂(OH), density functional theory (DFT) calculations and negative-ion mode electrospray mass spectrometer (ESI-MS) revealed that NHC tended to dissociate from the Pd(II), implying the succeeding generation of Pd(0)-PAR₂(O⁻) active species. Compared to Pd(0)-SPhos and Pd(0)-NHC, the oxidative addition of 4-chlorobenzonitrile to Pd(0) was computed, showing the Pd(0)-PAR₂(O⁻) has the lowest activation free energy. Ongoing work will be focused on the universality of NAPA in catalyzing cross-coupling reactions.

Keywords: heteroleptic palladium precatalysts, N-heterocyclic carbene, phosphinous acid, cross-coupling reactions, density functional calculation, mass spectrometry



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DESIGN, SYNTHESIS, AND SELECTIVE CYTOTOXICITY OF NOVEL ANTI-CANCER AGENTS TARGETING METASTATIC AND NON-METASTATIC BREAST CANCER CELLS

Emmanuel C. Ohaekenyem^{1*}, Jonathan I. Achika², Sunday E. Atawodi³, Ikenna Onyido¹, Samantha Loggenberg⁴, Jacqueline Maphutha⁴, Rochelle de Kock⁴, Frikkie Malan⁵, Namrita Lall^{4,6,7}

¹Pure and Industrial Chemistry Department Nnamdi Azikiwe University Awka, Nigeria.

²Department of Chemistry, Faculty of sciences, Federal University Lokoja, Kogi state, Nigeria

³Department of Biochemistry, Federal University of Lokoja, Kogi State, Nigeria

⁴Department of Plant and Soil Sciences, University of Pretoria, Pretoria, Gauteng, South Africa

⁵Chemistry Department, University of Pretoria, Pretoria, Gauteng, South Africa

⁶College of Pharmacy, JSS Academy of Higher Education and Research, Mysuru, India

⁷Senior Research fellow, Bio-Tech R&D Institute, University of the West Indies, Kingston, Jamaica

*Corresponding author: ec.ohaekenyem@unizik.edu.ng

Abstract

This study describes the synthesis and characterization of novel Fe, Ni, and Zn complexes derived from the 2,9-dimethyl-1,10-phenanthroline (dmp) ligand. The complexes were characterized by NMR spectroscopy, LC-MS, and XRD analysis. Additionally, their antioxidant properties were evaluated using the NO-scavenging assay. In vitro cytotoxicity assays were conducted on human breast cancer cell lines (MCF-7 and MDA-231-10A) and normal cells (HEK293) to assess the anticancer potential of the complexes. The results demonstrated that the Fe, Ni, and Zn complexes exhibited significant cytotoxic activity against both metastatic (MDA-231-10A) and non-metastatic (MCF-7) breast cancer cell lines. Notably, the complexes displayed selectivity towards cancer cells, exhibiting minimal toxicity towards normal HEK293 cells. Specifically, the Fe complex displayed IC₅₀ values of 7.06 ± 0.63 µg/ml and 4.149 µg/ml against MCF-7 and MDA-231-10A cells, respectively, with corresponding selectivity indices (SI) of 0.72. The Ni complex exhibited IC₅₀ values of 3.67 ± 0.67 µg/ml and 3.701 µg/ml against MCF-7 and MDA-231-10A cells, respectively, with corresponding SI values of 1.24. The Zn complex demonstrated IC₅₀ values of 1.81 ± 0.33 µg/ml and 2.407 µg/ml against MCF-7 and MDA-231-10A cells, respectively, with corresponding SI values of 1.99. To gain insights into the potential mechanisms of action, in silico studies were performed to investigate drug-drug interactions (DDI), protein-protein interactions (PPI), and molecular docking of the complexes. These analyses revealed potential interactions with key cancer-related proteins, suggesting that the complexes may exert their anticancer effects through multiple pathways. The findings of this study highlight the promising potential of Fe, Ni, and Zn complexes of the dmp ligand as novel anticancer agents. Further investigations are warranted to elucidate the precise mechanisms of action and to evaluate their efficacy in preclinical and clinical settings.

Keyword: 2,9-dimethyl-1,10-phenanthroline, Breast Cancer, Nitric Oxide Assay, In silico assay, Metal complexes

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COPPER SINGLE-ATOM NANOZYME MIMICKING GALACTOSE OXIDASE WITH SUPERIOR CATALYTIC ACTIVITY AND SELECTIVITY

Eslam Hamed¹, Limo He¹, Varun Rai², Song Hu³, Sam Li^{1*}

¹Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543, Singapore

²Department of Chemistry, Faculty of Science, University of Allahabad, Prayagraj, Uttar Pradesh, 211002, India

³State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan, 430074, China

*Corresponding author: chmlifys@nus.edu.sg

Abstract

Due to the low stability and high cost of some natural enzymes, nanozymes have been developed as enzyme-mimicking nanomaterials. Single-atom nanozymes are a class of nanozymes with metal centers that mimic the structure of metal-based natural enzymes. Herein, Cu-N-C single-atom nanozyme (SAN) was synthesized with excellent peroxidase- and enhanced oxidase-like activities to mimic the action of natural galactose oxidase. Cu-SAN demonstrates stereospecific activity akin to that of natural galactose oxidase by oxidizing D-galactose and primary alcohol but not L-Galactose or other carbohydrates. The SAN can catalyze the oxidation of galactose in the presence of oxygen, producing hydrogen peroxide as a sub-product. The produced hydrogen peroxide then oxidizes 3,3',5,5'-tetramethylbenzidine catalyzed by the SAN, yielding the typical blue product. The relationship between absorbance and galactose concentration was linear in the 1-60 μM range with a detection limit as low as 0.23 μM . This strategy can be utilized in the diagnosis of galactosemia disorder and detection of galactose in some dairy and other commercial products. Density functional theory (DFT) calculations clarify the high activity of the Cu sites in the peroxidase-like reaction and explain the selectivity of the Cu-SAN oxidase-like reaction toward D-galactose.

Keywords: Single-atom; Nanozyme; Galactose oxidase; Peroxidase; Catalysis

Graphic / Image



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INVESTIGATION OF Cu/ZnO CATALYSTS ON ADVANCED POROUS SUPPORTS FOR CO₂ TO METHANOL CONVERSION

Nor Hafizah Berahim^{a,*}, Akbar Abu Seman^a, Nor Hafizah Yasin^a

^aPETRONAS Research Sdn. Bhd.

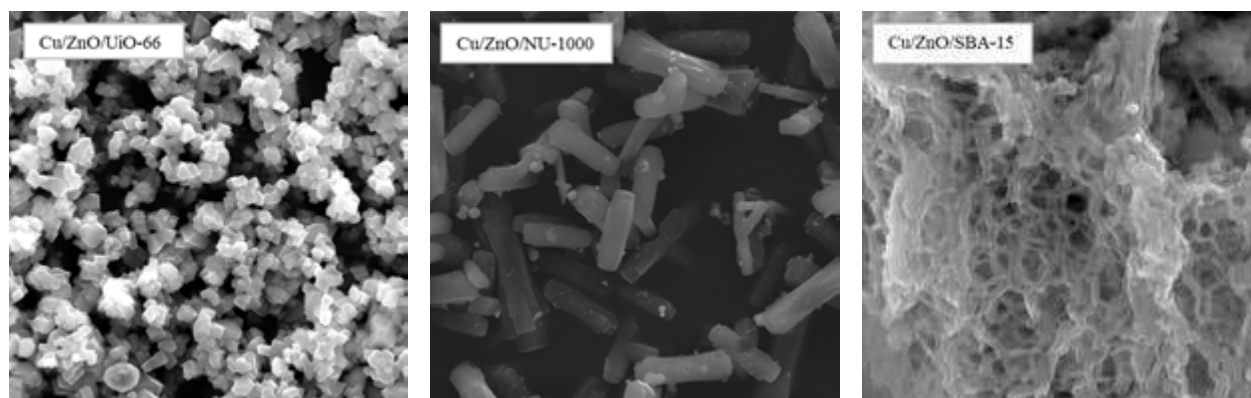
*Corresponding author: hafizah.berahimjusoh@petronas.com

Abstract

Rapid economic development driven by fossil fuel has caused a significant rise in CO₂ emissions, leading to global challenges like climate change, rising sea levels, and melting Arctic ice¹. To address this, there is increasing interest in converting CO₂ into useful products, particularly methanol through hydrogenation. Methanol, a key industrial chemical, offers potential as an eco-friendly fuel, capable of reducing both air pollutants and CO₂ emissions². However, the direct hydrogenation of CO₂ to methanol remains inefficient, requiring advanced catalysts and optimal conditions. The widely used Cu/ZnO/Al₂O₃ catalyst faces limitations, prompting research into modified catalysts, activators, and support materials to enhance performance and stability. Developing a more efficient process is essential for effective CO₂ utilization and environmental protection. The study highlights the catalytic conversion of CO₂ to methanol using Cu/ZnO supported on MOFs and SBA-15 and its physicochemical properties. The catalysts were synthesized via impregnation technique and characterized for X-ray diffractogram (XRD), field emission scanning electron microscopy (FESEM), and N₂-adsorption desorption. The performance of the synthesized catalysts were evaluated in a sealed batch reactor. The experimental findings indicate that the MOF catalysts outperformed the SBA-15 Cu/ZnO in terms of catalytic activity and CO₂ conversion under the mild reaction conditions with a TOF 9.4 times larger than the SBA-15 Cu/ZnO after 5 hours, whilst remaining highly selective for methanol production at 85.5%.

Keywords: CO₂, methanol, catalyst, Cu/ZnO, MOF, support

Graphic / Image



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GOLD(I) AND GOLD(III) PHOSPHANE TELLURIDES: FROM BONDING TO σ -HOLE ACTIVATION

Juan Carlos Pérez-Sánchez, Carmen Ceamanos, Jorge Echeverría, Juan Vicente Alegre-Requena, Raquel P. Herrera, M. Concepción Gimeno*

Instituto De Síntesis Química Y Catalisis Homogenea (Csic-University Of Zaragoza)

*Corresponding author: *gimeno@unizar.es

Abstract

Tellurium has become a vital element in modern chemistry, yet it remains a rarity, exhibiting distinct behavior compared to its chalcogen counterparts. Its unique characteristics have driven advancements across various fields, such as catalysis, materials science, and electronics. Phosphane chalcogenides, $R_3P=E$ ($E = O, S, Se, Te$; $R = \text{alkyl or aryl}$), exemplify the versatile chemistry of group 16 elements. These compounds are notable for their diverse electronic and chemical properties. However, while phosphane oxides, sulfides, and selenides have been extensively studied, the coordination chemistry of phosphane tellurides remains an underexplored field.²

This study seeks to bridge these gaps by synthesizing and characterizing gold(I) and gold(III) complexes with $TeP(iPr)_3$ as a ligand. By carefully selecting ancillary ligands, including the highly sterically hindered N-heterocyclic carbene IDipp*, we successfully stabilized elusive cationic gold(I) complexes containing a terminal $TeP(iPr)_3$ ligand. Extensive spectroscopic analyses, including ^{125}Te NMR, along with theoretical calculations, provided insights into the intricate bonding interactions within these compounds, as well as the potential mechanisms for their decomposition pathways, enhancing our understanding of gold-tellurium reactivity. Notably, coordination to the gold center enhances the σ -hole on the tellurium atom, introducing a new mode of activation for chalcogen bond catalysis (Figure 1). In addition, we have synthesized gold(III) complexes that exhibit an unprecedented formal tellurium insertion into a P–Au bond, representing the first observed tellurium transfer from $TeP(iPr)_3$ to a gold(III) complex.

Keywords: Gold; Tellurium; Bonding; Mechanism; Chalcogen Bonding Catalysis

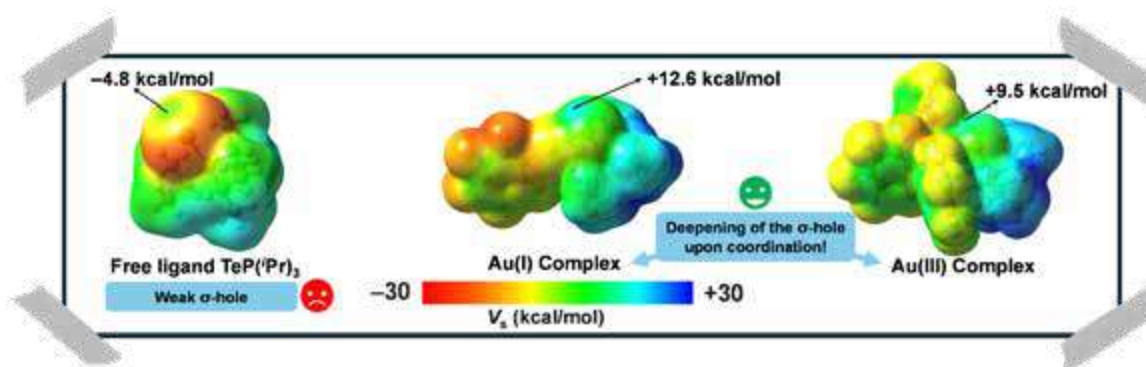


Figure 1. V_s , electrostatic potential on the molecular surface.

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NANOCATALYSTS AS ARTIFICIAL ENZYMES THEIR APPLICATIONS IN DIAGNOSTIC SYSTEMS

Sindisiwe Mvango^a, Simbongile Sicwetsha^a, Omotayo Adeniyi^a, Ridge Chavhalala^a,
Philani Mashazi^{a,b,*}

^aChemistry Department, ^bTebello Nyokong Institute for Nanotechnology Innovation.

*Corresponding author: p.mashazi@ru.ac.za

Abstract

Nanoscience brought about various interesting properties such as optical gold nanoparticles, catalytic palladium nanoparticles, magnetic iron oxide nanoparticles, and inert silica nanoparticles. These wide properties are still being explored for various applications. Diagnostic systems for communicable and non-communicable diseases are crucial in global health applications. In various research, we have explored their potential as biomimetics due to their excellent reactive oxygen radical species generation for disease biomarker detection. In our research, we have investigated several nanomaterials¹⁻⁴ as monometallic and bimetallic catalysts. Their investigation involved the evaluation as possible substitutes for natural enzymes. This has also been demonstrated in their applications in the design of biosensors for glucose detection^{1,2a,3a}, monitoring vitamin C (ascorbic acid)⁴, and anti-p53 autoantibodies as cancer disease biomarkers^{3b,c}. **Figure 1** shows a select few nanomaterials that have been prepared and evaluated their biomimetic properties. The presentation will show the intricate procedures for preparing nanomaterials with the aim of enhanced catalytic effect for biomimetic evaluations and some of the recent nanomaterials which showed excellent enzymatic properties.

Keywords: nanocatalysts, enzymatic properties, biomimetics, reactive oxygen species, disease biomarkers.

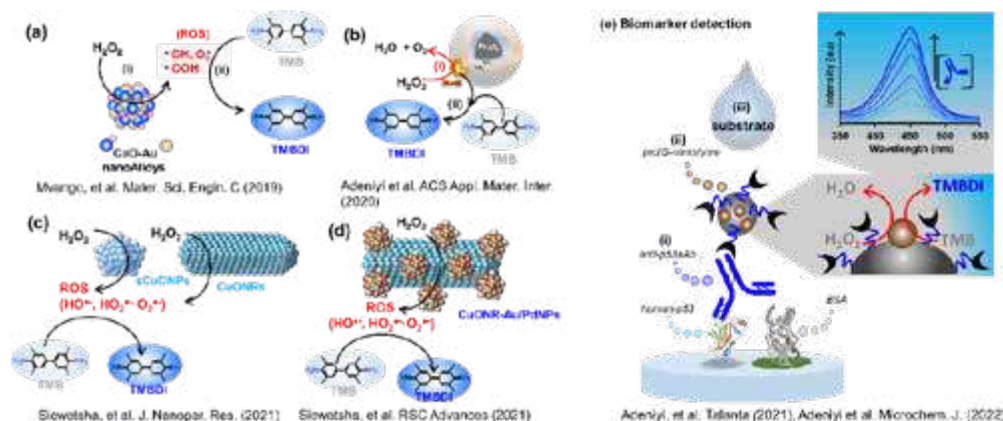


Figure 1: Nanoparticles (NPs) with enzyme-like catalysis (a) CuO-Au nanoalloys¹, (b) magnetic nanoparticles (NPs)^{2(a)}, (c) spherical and rod-like CuONPs^{3(a)}, (d) CuO nanorods decorated with Au@PdNPs^{3(b)}, and (e) nanozymes applied for the disease biomarker detection^{2(b),(c)}.

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DEVELOPING BIOORGANOMETALLIC COMPLEXES FOR CANCER AND MICROBIAL DISEASES

Prinessa Chellan,^{a*} Remofilwe Manye,^a Leandre van der Merwe,^a Stacey Roman^a

^a Department of Chemistry and Polymer Science, Stellenbosch University, Stellenbosch, Western Cape, South Africa

* Corresponding author: pchellan@sun.ac.za

Abstract

The investigation of novel metal complexes as therapeutics is a thriving area of research [1]. In particular, organometallic complexes have been intensely investigated for their inhibitory effects against cancer and different parasite and bacterial strains which has affirmed their prospective application as antimicrobials [2]. One popular approach to combat illnesses such as malaria or cancer, is the incorporation of a metal into currently used clinical drugs or known pharmacophores, thus modifying their biological activity [1]. In our research group, we currently investigate the organometallic derivatisation of two scaffolds with promising biological activities - benzimidazoles and artesunate.

In this presentation, I will discuss some of the latest work we have completed on new organometallic complexes with in vitro inhibitory activity for cancer and malaria [3, 4]. This includes research on drug delivery using polymer micelles for *Plasmodium falciparum*. The data supports the hypothesis that incorporation of organometallic groups influences biological activity, in vitro, and can potentially be correlated to the stability and reactivity of the metal complexes.

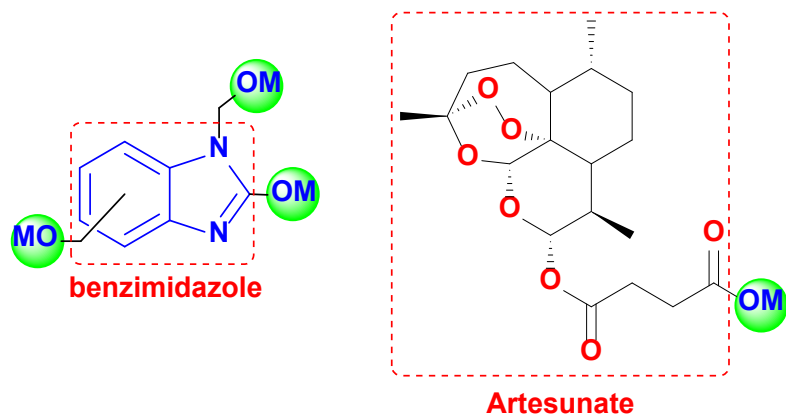


Figure 1. The benzimidazole and artesunate scaffolds of interest and the sites of organometallic derivatization. OM = organometallic (ferrocene or half sandwich Rh(III), Ir(III), Ru(II) moieties)

Keywords: Cancer, antimicrobial, organometallic

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METAL AMINO-BIS(PHENOLATE) COMPLEXES AS CATALYSTS FOR COPOLYMERIZATION OF CARBON DIOXIDE, EPOXIDES AND ANHYDRIDES

Christopher M. Kozak^{a*}

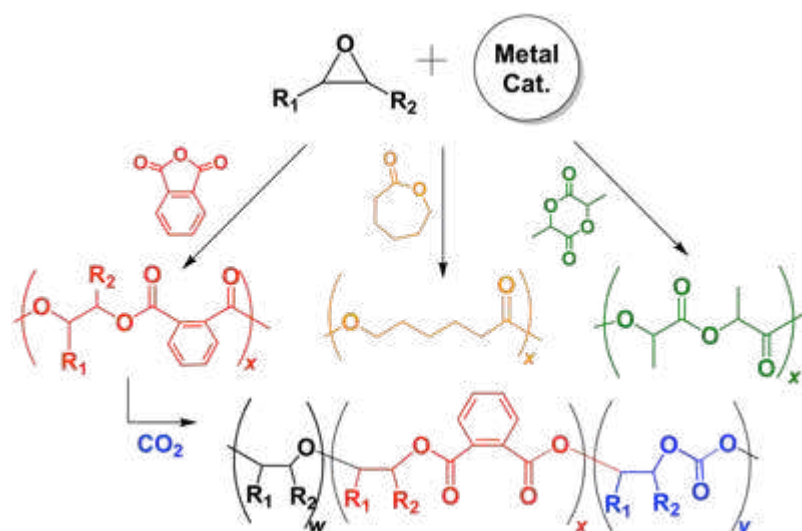
^aMemorial University of Newfoundland

*Corresponding author: ckozak@mun.ca

Abstract

Cyclic and polycarbonate synthesis from CO₂ and epoxides is a promising method of using CO₂ as a C-1 feedstock. Catalysts to-date have shown the breadth of active metal complexes include Zr, Cr, Fe, Co, Ni, Zn containing systems with diverse multidentate ligands. We have focused our attention on the amino-bis(phenolate) ligand framework, which is highly modifiable both sterically and electronically. These ligands can be paired with metals from across the periodic table including both main group and transition metals. This work will present a survey of comparable activities for early, mid and late transition metal complexes of amine-bis(phenolate) ligands for polymerization reactions of CO₂ with epoxides, as well as cyclic ester ring-opening polymerization and ring-opening copolymerization of epoxides with cyclic anhydrides. Mechanistic studies and kinetic data obtained by in situ IR spectroscopy will be discussed along with structure/activity relationships resulting from steric and electronic modification of the ligand systems.

Keywords: metal-catalyzed polymerization, epoxides, lactide, polyester, copolymers



FROM WASTE TO POWER: UTILIZING BARLEY HUSK AS A SUSTAINABLE ANODE ACTIVE MATERIAL ALTERNATIVE TO GRAPHITE IN LITHIUM-ION BATTERIES

Chenghao Yue^{a,b}, Alireza Fereydooni^{a,b,c}, Mingrui Liu^a, Yuexi Zeng^a, Zhijie Wei^a, Yimin Chao^{a,b,*}

^a National energy key laboratory for new hydrogen-ammonia energy technologies, Foshan Xianhu Laboratory, Foshan 528200, P. R. China

^b School of Chemistry, University of East Anglia, Norwich NR4 7TJ, UK

^c Tyndall Center for Climate Change Research, University of East Anglia, Norwich NR4 7TJ, UK *Corresponding
*Corresponding author: y.chao@uea.ac.uk

Abstract

The escalating concerns over global warming, the rapid depletion of fossil fuel reserves, and the pressing need to reduce carbon emissions in the electric power sector have intensified the focus on renewable energy sources.^{[1]–[3]} lithium-ion batteries (LIBs) have emerged as the leading solution due to their high energy density, long cycle life, and eco-friendliness.^{[6], [7]} Barley husks (BHs), an agricultural by-product rich in carbon and silica, were utilized as a sustainable precursor for synthesizing hard carbon anode materials for lithium-ion batteries (LIBs). A comparative analysis with graphite, the conventional anode material, demonstrates the potential of BH-derived carbon as a viable alternative. Material characterization techniques confirmed the formation of a hard carbon structure with a porous morphology, enhanced by the silica content, which contributes to structural stability and performance. The BHs-derived anode exhibited a specific capacity of at C/5, surpassing that of graphite, with improved cycling stability and rate capability. This material, derived from agricultural waste, presents a sustainable and promising alternative for next-generation energy storage technologies, with improved performance and eco-friendly potential.

Keywords: anode materials, lithium-ion batteries, hard carbon, silica, barley husks

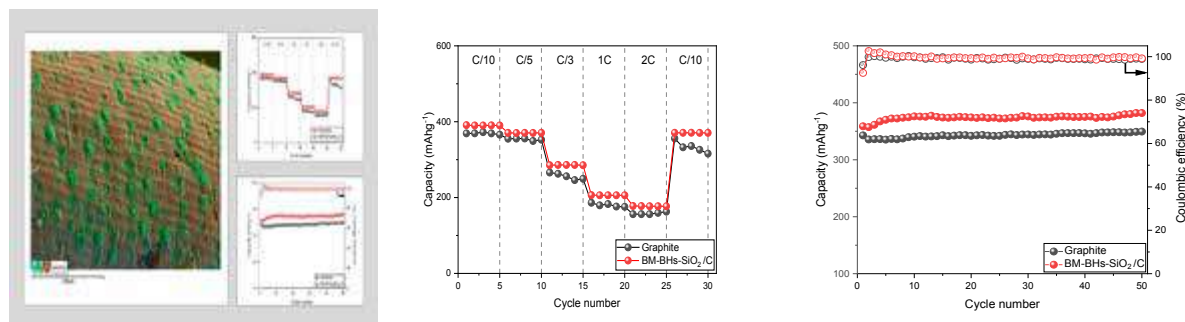


Figure 1. a) SEM image and EDX elemental mapping (Si, C, O) of BHs-SiO₂/C sample after acid wash, b) the rate performance, and c) cycling performance comparison of Graphite and BM-BHs-SiO₂/C

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OPTIMAL ELECTRONIC STRUCTURE OF Ru-BASED ELECTROCATALYSTS FOR HYDROGEN OXIDATION REACTION

Licheng Wei^{a*}

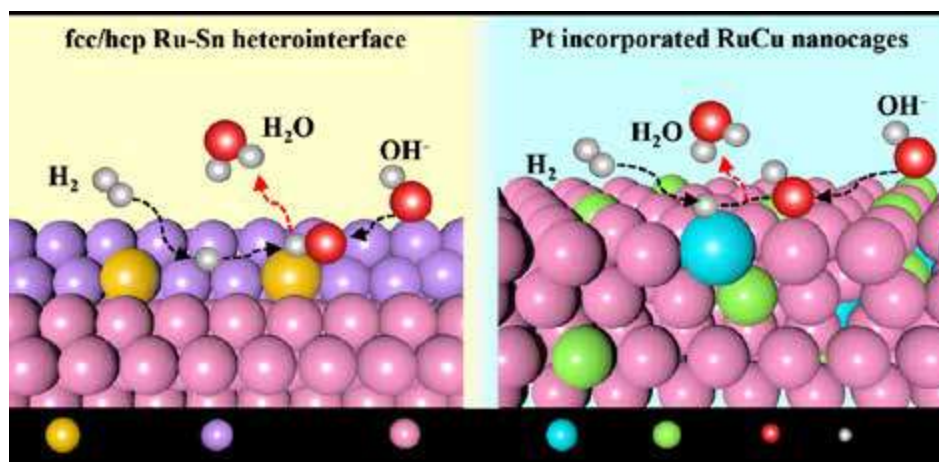
^aNational energy key laboratory for new hydrogen-ammonia energy technologies, Foshan Xianhu Laboratory,
1 Yangming Road, Foshan 528200, China

*Corresponding author: weilicheng@xhlab.cn

Abstract

Ruthenium (Ru)-based electrocatalysts have emerged as highly promising candidates for anode materials in anion exchange membrane fuel cells (AEMFCs), attracting considerable interest owing to their exceptional ability to enhance the kinetic rate of the hydrogen oxidation reaction (HOR). Our research focuses on optimizing the electronic structure of Ru-based electrocatalysts to mitigate the adsorption of intermediates (H^*/OH^*) and thereby enhance the performance of HOR, aligning with the requirements of AEMFCs. Initially, we developed an fcc/hcp heterointerface of Ru-Sn by introducing the metalloid element of Sn to rearrange the charges distribution at the heterointerface, thereby alleviating the H^* adsorption energy on Ru sites.¹ Subsequently, we observed a sudden decline in the catalytic activity of Ru-Sn dropped at elevated potential, which might be attributed to the strong interaction between Ru sites and hydroxide species. Consequently, we fabricated hollow RuCu nanocages with a limited incorporation of Pt, leading to an electron-rich Ru and a lowered d -band center, which facilitates the reduction of interactions between active sites and OH^* , accelerates the migration rate of OH^* and H^* , and enhances the reaction kinetics of HOR.² As a result, the aforementioned electrocatalysts, optimized through the incorporation of heteroatoms, demonstrate improved specific peak power density performance of AEMFCs, offering a valuable reference for the design of efficient Ru-based electrocatalysts applicable to HOR and AEMFCs.

Keywords: hydrogen oxidation reaction, intermediates adsorption, electronic structure, heterointerface



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DEVELOPMENT OF GOLD-BASED ORGANOMETALLIC COMPOUNDS AS POTENTIAL ANTICANCER AGENTS

Katleho Setlaba ^{a,*}, Vuyo Mavumengwana ^b, Prinessa Chellan ^a

^a Department of Chemistry and Polymer Science, Stellenbosch University, Stellenbosch, Western Cape, South Africa

^b Division of Molecular Biology and Human Genetics, Biomedical Research Institute (BMRI), Tygerberg, Cape Town, Western Cape, South Africa

* Corresponding author: 20323891@sun.ac.za

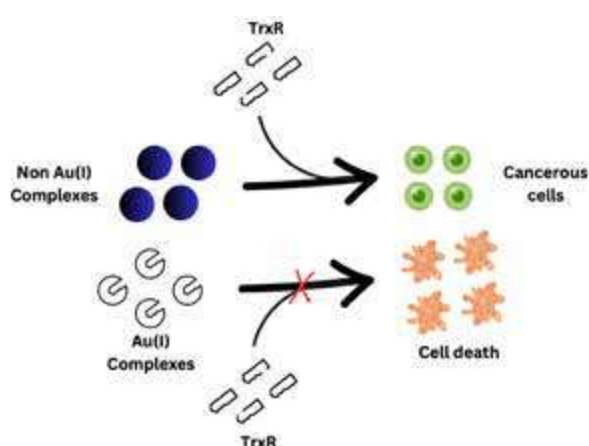
Abstract

Cancer remains a leading global health disease, accounting for nearly 10 million deaths in 2022.^[1] While chemotherapy has revolutionized cancer treatment, there continues to be challenges including toxicity, drug resistance, and systemic adverse effects. Thus, there is an urgent and continual need for innovative therapeutic agents.^[2]

Gold(I) complexes have emerged as promising candidates, offering exceptional stability, low toxicity, and selective biomolecular interactions.^[3] Unlike cisplatin, which disrupts DNA repair, gold compounds target specific pathways, primarily the thioredoxin reductase (TrxR) system.^[3] TrxR, a central regulator of cellular redox homeostasis, catalyses NADPH-dependent reduction of oxidized thioredoxin (Trx). By inhibiting TrxR, gold(I) complexes induce oxidative stress, disrupt redox signalling, and trigger apoptosis.^[3] This mechanism circumvents classical resistance pathways, making TrxR a promising therapeutic target.

Critical to the efficacy of gold(I) complexes is their stability under physiological conditions. Strong metal-ligand bonds are essential for ensuring intact delivery to target sites. *N*-heterocyclic carbenes (NHCs) exhibit exceptional σ -donor strength, while their tuneable steric and electronic properties enable precise optimization for biological compatibility.^[4] Furthermore, their ease of synthesis allows functionalization with hydrophilic, hydrophobic or targeting groups, enhancing bioavailability and tumour specificity.^[4] In this presentation, we will discuss the synthesis and characterisation of new Au (I) organometallic complexes and their ability to selectively disrupt cancer cell mechanisms while minimizing off-target effects.

Keywords: Cancer, Gold complexes, *N*-heterocyclic carbenes, Thioredoxin reductase, Resistance



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EXPLORING THE ANTICANCER POTENTIAL OF ORGANOMETALLIC PGM COMPLEXES CONTAINING SELECTED INDOLE DERIVATIVES

Brandon Munnik^{a,*}, Prinessa Chellan^a

^a Department of Chemistry and Polymer Science, Stellenbosch University, Stellenbosch, Western Cape, South Africa

*Corresponding author: 19773544@sun.ac.za

Abstract

Cancer remains a global threat, with the most up to date data from the World Health Organization (WHO) reporting approximately 20 million new cases and 10 million deaths in 2022.¹ Despite severe side effects and development of resistance, platinum-based chemotherapeutic agents are still widely used in the treatment of various cancers.² Our group focuses on a targeted approach by combining platinum-group metals to organic pharmacophores with the intent of reducing side effects by targeting proteins which enable the growth and development of cancer. One such target is the chaperone protein Heat Shock protein 90 (HSP90), which plays a role in the growth and metastasis of cancer cells.³ β -carboline and their derivatives have shown promising results in the treatment of cancer as well as the ability to target this group of proteins.^{4,5} Thus, in this presentation, the design and development of novel half-sandwich metal complexes of tetrahydro- β -carboline derivatives and the determination of their anticancer activities will be discussed. Molecular docking was used to determine the interactions between the complexes and the N-terminal of the *Homo sapiens* HSP90 known for being the active site of many drug targets.

Keywords: Organometallic, Indole derivatives, Cancer, Molecular docking, Heat shock proteins

Graphic / Image

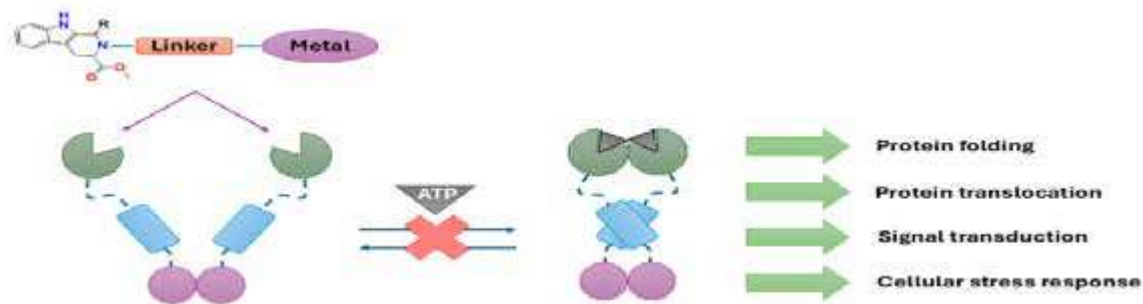


Figure 1: Potential mode of action for synthesized bioorganometallic drugs.

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PHOTOCATALYTIC APPLICATION OF MONODISPERSE CLUSTER-BASED MULTI-LEVEL STRUCTURAL MATERIALS

Shi wenxiong^{*1}

¹ Institute for New Energy Materials and Low Carbon Technologies, School of Materials Science & Engineering,
Tianjin University of Technology, Tianjin 300384, China,

*Email: wxshi@email.tjut.edu.cn

Abstract

Monoatomic catalysts have attracted extensive attention in the field of catalysis because of their high atomic utilization rate. The synthesis of monoatomic catalysts has made great progress, however, it is still challenging to accurately characterize the fine structure of monoatomic sites according to ligand elements and spatial configuration. The high surface energy of a single atom usually leads to aggregation into nanoclusters or nanoparticles, which significantly reduces the utilization efficiency of atoms. Therefore, it is very important to select suitable carriers to firmly fix a single metal center and prepare monoatomic catalysts with precise structures.

Polyoxometallate (POM) clusters have definite composition, precise structure and ultra-fine size, and their diversified structures are easy to design and control, and they have good photoelectric sensitivity and redox property, and can also be used as carriers to support various catalytic active centers. Site substitution or surface modification of POM can form strong interaction between nano clusters, and the assembly behavior of POM clusters can be dominated by regulating the force at the single molecule level. Therefore, according to its own spatial structure characteristics and combined with ligands such as surfactants and counterions, directional assembly can be designed to obtain highly ordered multi-level structural materials. Therefore, it has great potential in the design and preparation of catalysts to construct well-defined multi-level structural materials by dispersing single metal-substituted POM clusters.

Design, synthesis, assembly and preparation of multilevel structural materials based on POM clusters combined with multi-scale research can explore the assembly mechanism, dispersion effect and synergistic catalysis of multilevel structural materials. The dynamic model of sub-nano clusters can be established by quantitative calculation combined with classical force field and experimental characterization parameters. By adjusting the proportion and types of POM, ion and ligand, multi-level complex structures¹⁻⁵ can be obtained by assembly and evolution respectively. This method can reveal the basis and evolution law of monodisperse monoatomic cluster multilevel structure materials at the atomic level, and prepare monodisperse functional cluster-based materials and devices.

Keywords : Cluster ; Polyoxometallate; Monodisperse; Multilevel structural materials; Photocatalysis

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PT(II) COMPLEXES WITH BIDENTATE (IMINO)PYRIDINE: SYNTHESIS, CHARACTERIZATION, REACTIVITY TOWARDS THIOL, DNA INTERACTIONS AND CYTOTOXICITY STUDIES

Mangaliso Goge^a, Tshephiso Papo^{a,*}, Siphamandla Sithebe^a

^a*School of Chemistry and Physics, University of KwaZulu-Natal, South Africa, Scottsville, 3209*

**Corresponding author: papot@ukzn.ac.za*

Abstract

Several Pt(II) complexes have been explored for their cytotoxic properties in the pursuit of alternate anticancer drugs due to the development of resistance to traditional platinum-based drugs.¹ Numerous anticancer drugs have been studied and reported over the years to develop less toxic, but equally effective complexes as the well-known cisplatin. This study investigates the steric and electronic effects of bidentate (imino)pyridine Pt(II) complexes by exploring their DNA interactions, substitution kinetics, and cytotoxicity. The (imino)pyridine ligands **L1** to **L4** and their corresponding platinum (II) complexes, viz. dichloro(N-isopropyl-2-picolinaldimine)platinum(II) (**PtL1**), dichloro[N-(2-pyridinylmethylene)benzenamine-N,N']-platinum(II) (**PtL2**), dichloro[2,6-dimethyl-N-[(2-pyridinyl)methylene]benzenamine-N,N']-platinum(II) (**PtL3**) and dichloro[2,6-bis(1-methylethyl-N-[(2-pyridinyl)methylene]benzenamine-N,N']-platinum(II) **PtL4**, were synthesized and characterized using NMR (¹H & ¹³C), mass spectrometry, FT-IR, elemental analysis, and UV-Visible spectrophotometry. Single crystal X-ray crystallography was further used to elucidate the structure of **PtL1**, **PtL2**, and **PtL3**. **PtL1** and **PtL2** crystallized in the monoclinic systems with *P2₁/n* and *P2₁/n* space groups, respectively, while **PtL3** crystallized in the triclinic crystal system with the *P-1* space group. The coordination geometry around the platinum atom in all three complexes exhibited a distorted square planar geometry. The substitution behaviour of coordinated chloride atoms by a bio-relevant nucleophile, Tu, was studied in a 0.1 M LiCl solution under *pseudo*-first-order conditions using UV-visible spectrophotometer. The reactivity of the Pt(II) complexes is influenced by the electronic and steric effects of the coordinated ligands. The interactions of the complexes with ct-DNA showed that these metal compounds are possible partial intercalators with intrinsic binding constants in the order of 10⁵ M⁻¹. Cytotoxic studies of the complexes with HeLa and HEK293 cell lines revealed that **PtL1** was the most potent against HeLa cell lines, and **PtL2** had the highest activity towards HEK293 cell lines, with IC₅₀ values at 6.67x10⁻⁸ and 3.93x10⁻⁶ μM, respectively.

Keywords: Platinum, substitution, cytotoxicity, ctDNA

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SURFACE ORGANOMETALLIC CHEMISTRY FOR SINGLE-ATOM CATALYSIS

Pengxin Liu^{a,*}

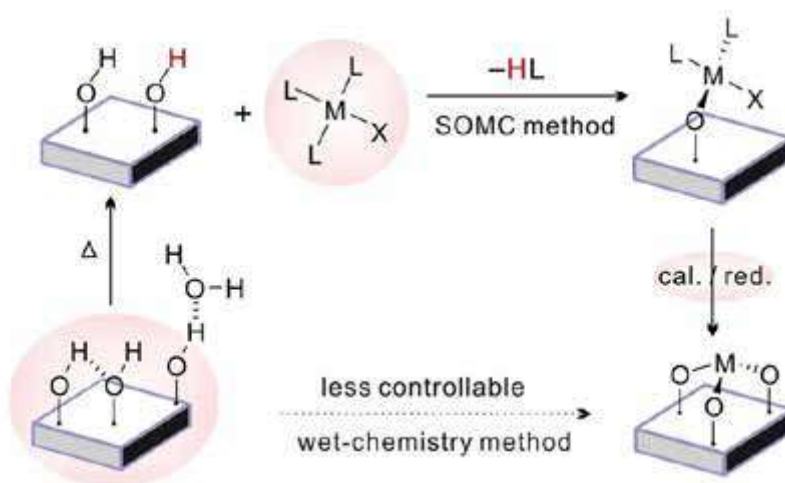
^a*School of Physical Science and Technology, ShanghaiTech University, Shanghai, P. R. China*

**Corresponding author: liupx@shanghaitech.edu.cn*

Abstract

Although extensive efforts have been made to bring homogeneous and heterogeneous catalysis closer, the gap between these two research fields still stands. Surface organometallic chemistry (SOMC) method has been developed along with organometallic chemistry and surface science from the 1970s. We showed that applying SOMC on single-crystalline MgO(111) two-dimensional nanosheets is an ideal way to prepare single atom catalysts with uniform catalytic sites with identical coordination structures, for fundamental interests. The single crystallinity of the support, the exposed ordered crystalline planes and the SOMC method are ideally suited to minimize the surface heterogeneity for anchoring atomically dispersed species.

Keywords: Surface organometallic chemistry; Single-atom catalyst; Single-site catalyst; Surface coordination chemistry; 2D material;



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DEVELOPMENT OF $\text{Fe}_3\text{O}_4/\text{ZnO}$ HETEROSTRUCTURE PHOTOCATALYST DERIVED FROM FE-DOPED ZIF-8 FOR THE PHOTOCATALYTIC DEGRADATION OF TETRACYCLINE AND HYDROGEN PEROXIDE PRODUCTION

Sumiyyah Sabar^{a*}, Afiqah M. Jamil^a, Yifan Zhao^b, Enis Nadia Md Yusof^a, Raphaël Schneider^c, Abdul Rahman Mohamed^d, Yasutaka Kuwahara^{b,e}, Kohsuke Mori^{b,e}, Hiromi Yamashita^{b,e}

^aChemical Sciences Programme, School of Distance Education (SDE), Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

^bDivision of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

^cUniversité de Lorraine, CNRS, LRGP, F-54000 Nancy, France

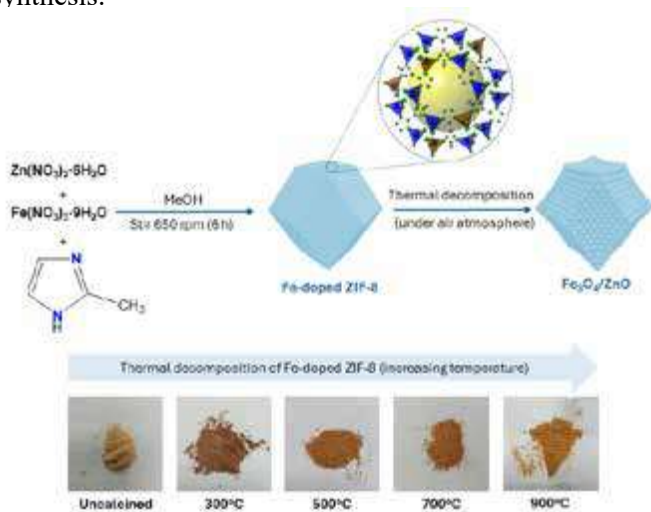
^dSchool of Chemical Engineering, Universiti Sains Malaysia, Engineering Campus, Nibong Tebal, Pulau Pinang 14300, Malaysia

^eInnovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (OTRI), Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

*Corresponding author: sumiyyahs@usm.my

Abstract

This research investigates the development of $\text{Fe}_3\text{O}_4/\text{ZnO}$ heterostructures derived from Fe-doped ZIF-8 via a combined precipitation and thermal decomposition method. Fe^{3+} ions were successfully introduced into the ZIF-8 framework, partially substituting Zn^{2+} ions to facilitate in the formation of $\text{Fe}_3\text{O}_4/\text{ZnO}$ heterostructures upon calcination under air. Comprehensive analyses using ultraviolet-visible diffuse reflectance spectroscopy (UV-Vis DRS), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) verified the formation of these crystalline heterostructures. Enhanced visible-light absorption, a reduced bandgap, and defect state generation were observed, which promoted improved charge separation and reduced recombination rates of electron-hole pairs. The photocatalytic performance of these heterostructures were evaluated through the degradation of tetracycline (TC) and production of hydrogen peroxide (H_2O_2) under visible light irradiation. Notably, heterostructures derived from Fe-ZIF-8 calcined at 500°C exhibited superior photocatalytic activity, degrading 74.8% of TC in 2 hours and producing $919.2\ \mu\text{M}$ of H_2O_2 in 3 hours. Superoxide radicals ($\cdot\text{O}_2^-$) were identified as the dominant reactive species in these processes. The findings demonstrate the potential of these ZIF-8-derived photocatalysts for environmental remediation and green chemical synthesis.



Keywords: metal-organic frameworks, doping, heterostructures, thermal decomposition, photocatalysis.

AMORPHOUS CATALYSTS FOR CO₂ ELECTROCATALYSIS AND SELECTIVE FORMATION OF C1 AND C2 PRODUCTS

Akshayini Muthuperiyanayagam^a, Devis Di Tommaso^{a,b,*}

^a Department of Chemistry, School of Physical and Chemical Sciences, Queen Mary University of London, Mile End Road, London, E1 4NS, United Kingdom

^b Digital Environment Research Institute, Queen Mary University of London, Empire House, 67-75 New Road, London E1 1HH, UK

*Corresponding author: d.ditommaso@qmul.ac.uk

Abstract

The conversion of CO₂ into value-added chemicals offers a promising solution to mitigate rising global CO₂ emissions and promote sustainable environmental practices.¹ cement manufacturing, and chemical production. Carbon capture utilization and storage (CCUS) We present a computational study combining machine learning force fields and DFT calculations to explore amorphous copper (Cu)² and copper-nickel (CuNi) as catalysts for the CO₂ electrochemical reduction (CO₂R) to C1 and C2 products. Our findings show that amorphous Cu and CuNi surfaces, unlike their crystalline counterparts, provide a broader range of coordination environments (Fig 1(c-f)), creating multiple active sites for CO₂ adsorption. This structural flexibility enables tuning of product selectivity through various reaction sites. Moreover, both amorphous Cu and CuNi surfaces spontaneously activate CO₂, indicating their potential for efficient conversion. Specifically, amorphous CuNi catalysts demonstrate higher selectivity for CO₂ reduction to ethanol over ethylene compared to crystalline CuNi catalysts (Fig 1g). This enhanced selectivity is attributed to the unique coordination sites on the amorphous surface. The stability of CO₂R intermediates are significantly improved, resulting in lower overpotentials and better selectivity. These findings emphasize the advantages of amorphous catalysts in CO₂ reduction, offering a promising approach for designing catalysts with tailored selectivity. This study provides a basis for further exploration of amorphous Cu-based catalysts in sustainable CO₂ conversion, highlighting their promising potential to support climate change mitigation strategies.

Keywords: Electrochemical CO₂ reduction, amorphous Cu-based catalysts, density functional theory, machine learning forcefields, and tunable product selectivity.

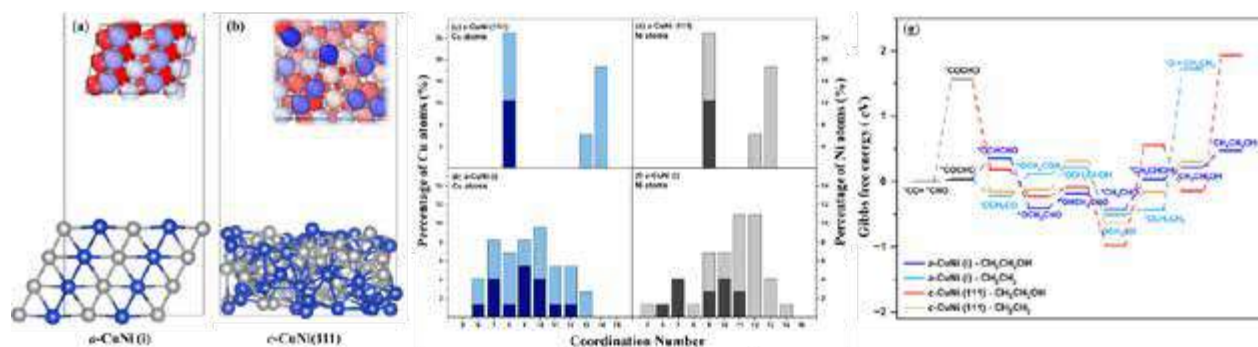


Figure 1: (a-b) Cu-based amorphous catalysts, (c-f) catalyst coordination number analysis and (g) electrochemical CO₂ reduction to C2 products

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BACTERIAL METALLOPROTEINASES AS VIRULENCE FACTORS: EXPLORING PEPTIDE-BASED INHIBITION

Martyna ZAWADA^a, Paulina POTOK^a, Sławomir POTOCKI^{a*}

^aFaculty of Chemistry, University of Wrocław, 50-383 Wrocław, Poland;

*Corresponding author: slawomir.potocki@uw.edu.pl

Abstract

The growing threat of antibiotic resistance has made bacterial infections harder to treat, necessitating novel therapeutic approaches.¹ Among key bacterial virulence factors, metalloproteinases (MPs) from the M4 and M10 families play crucial roles in host tissue degradation and immune evasion. Their Zn(II)-dependent activity makes them attractive targets for inhibition.²

In this study, we investigated MPs from antibiotic-resistant strains, focusing on their metal coordination chemistry. We explored the competitive binding of Zn(II) and Cu(II), assessing whether copper could displace zinc and inhibit enzymatic function. Site-directed mutagenesis helped identify key residues essential for metal coordination.³ Additionally, we designed substrate-based peptide inhibitors that mimic natural substrates, enhancing selectivity and pharmacological potential (Fig. 1).⁴

To characterize metal-ligand interactions and inhibitor binding, we employed mass spectrometry, NMR spectroscopy, UV-Vis spectroscopy, and circular dichroism. These analyses provided valuable insights into the molecular interactions of transition metal ions with protein metal-binding domains and inhibitors. By characterizing these interactions, our findings contribute to understanding the specificity of metal coordination and its role in enzymatic inhibition. This work lays the foundation for designing more selective and effective therapeutics against antibiotic-resistant pathogens.

Keywords: coordination chemistry, metalloproteinase, inhibition, antibiotic resistance

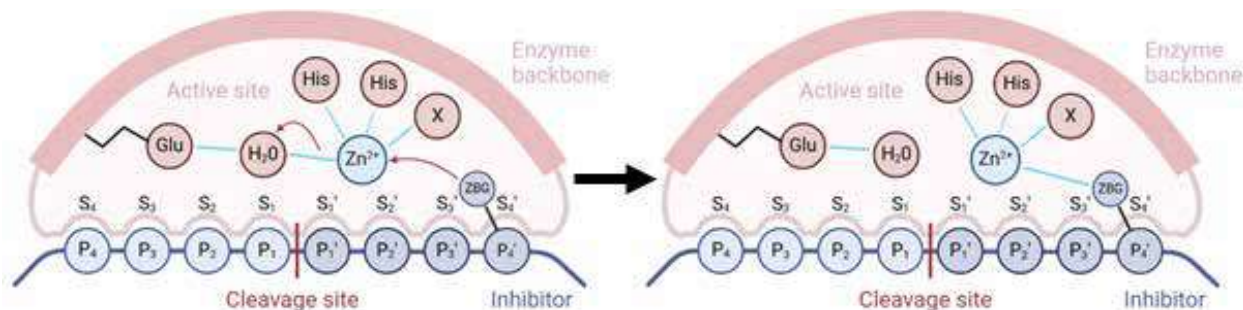


Figure 1: Mechanism of inhibition by a substrate-mimicking inhibitor. The inhibitor binds to the active site via a zinc-binding group (ZBG), preventing substrate cleavage and release.⁵

Financial support by the National Science Centre (UMO-2023/50/E/ST5/00434) is gratefully acknowledged.

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MODELLING THE CATALYTIC DOMAIN OF BACTERIAL VIRULENCE FACTORS: A FIRST STEP TOWARDS INHIBITOR DESIGN

Paulina Potok^a, Arian Kola^b, Daniela Valensin^b, Merce Capdevila^c, Slawomir Potocki^{a*}

^aFaculty of Chemistry, University of Wrocław, 50-383 Wrocław, POLAND

^bDepartment of Biotechnology, Chemistry and Pharmacy, University of Siena, 53100 Siena, ITALY

^cDepartment of Chemistry, Universitat Autònoma de Barcelona, 08193 Cerdanyola del Vallès, SPAIN

*Corresponding author : slawomir.potocki@uwr.edu.pl

Abstract

The increasing spread of antibiotic resistance among bacterial pathogens is a major global health concern. A promising approach for developing new antibiotics involves targeting bacterial virulence factors, such as metalloproteases (MPs)—proteolytic enzymes that use metal ions, primarily Zn(II), to catalyze hydrolytic reactions. Since MPs play a critical role in infection processes, understanding their coordination chemistry is essential for designing therapeutics that inhibit activity. However, determining enzyme structures using traditional methods can be complex, time-consuming, and costly. Peptides derived from protein binding sites offer effective protein mimetic models that provide insights into enzyme-inhibitor interactions, facilitating drug design.

This study investigated the coordination chemistry of Zn(II) and Cu(II) ions within the catalytic domains of MPs from multidrug-resistant bacteria, including AprA from *Pseudomonas aeruginosa*, CpaA from *Acinetobacter baumannii*, and M10 from *Streptococcus pneumoniae*^{1,2,3}. The analysis identified distinct coordination patterns of Zn(II) and Cu(II) ions within the conserved HExxHxxxxxH motif at pH levels below 7^{1,2}. Among the examined systems, the peptide model of CpaA exhibited the highest thermodynamic stability for both Zn(II) and Cu(II) complexes. Non-coordinating amino acids surrounding the metal center in CpaA enhanced complex stability through intramolecular interactions, which also facilitated the formation of the left-handed polyproline II helix (PPII)—a rare protein structure associated with protein-protein and protein-ligand interactions³.

This study expands the understanding of the coordination properties of Zn(II)- and Cu(II)-MP complexes, providing detailed physicochemical, structural, and thermodynamic data. These findings offer a foundation for future research on interactions between MPs' catalytic domains and potential inhibitors, supporting the development of novel antimicrobial agents.



Keywords: coordination chemistry, bioinorganic chemistry, metal complexes, peptides, zinc

Financial support by the National Science Centre (UMO-2023/50/E/ST5/00434) is gratefully acknowledged.

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INVESTIGATING THE PHYSICOCHEMICAL PROPERTIES AND BIOLOGICAL INTERACTIONS OF NOVEL NI(II), PD(II), AND PT(II) METALLODRUGS

Sheldon Sookai^a, Ayanda Majoka^a, Manuel A. Fernandes^a, Monika Nowakowska^{*a}

^aMolecular Sciences Institute, School of Chemistry, University of the Witwatersrand, South Africa

*Corresponding author: Monika.nowakowska@wits.ac.za

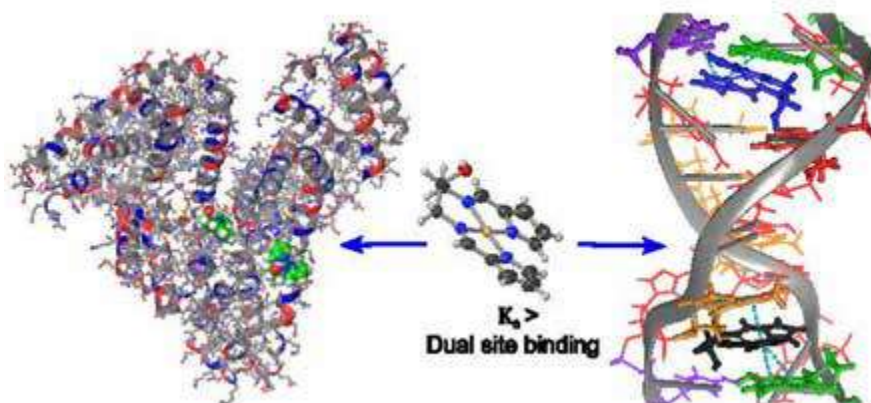
Abstract

The development of novel metallodrugs necessitates a comprehensive evaluation of their physicochemical properties and biological interactions, such as: (i) whether the metallodrug remains intact and what species are present at different pH levels, (ii) the stability of the drug in serum and its components, (iii) a proposed mode of action (MOA), such as its interaction with DNA, and (iv) monitoring its binding to human serum albumin (HSA), the most abundant blood protein responsible for transporting many exogenous compounds.

In this study, Ni(II), Pd(II) and Pt(II) chelates of a tetradentate 1,3-bis(((E)-(1H-pyrrol-2-yl) methylene) amino) propan-2-ol ligand, H2L, were synthesized and assessed for their stability at varying pH levels and in human serum. Spectroscopic techniques, including fluorescence and UV-CD spectroscopy, were used to investigate the interactions of the metal chelates with DNA and human serum albumin (HSA) under physiological conditions. Complementary in silico methods were then utilized to corroborate the experimental data and provide molecular insights into the binding mechanisms.

The spectroscopic and in silico results, highlighting a systematic approach to evaluating the physicochemical properties and biological interactions of novel metallodrugs will be discussed, thus contributing to the rational design and development of effective metallodrugs with potential therapeutic applications.

Keywords: Metallodrugs, HSA, ctDNA, spectroscopy, molecular dynamics



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ATOMICALLY PRECISE INORGANIC HELICES WITH A PROGRAMMABLE TWIST

Maxx Q. Arguilla^{a,*}

^aUniversity of California, Irvine

*Corresponding author: marguill@uci.edu

Abstract

The complex chiral nature of helical structures endows materials that display these motifs with unusual physical and quantum properties. Yet, as ubiquitous as it is in nature and engineered organic systems, there has been a dearth of dense inorganic solids that manifest helicity across extended lattices—where these emergent properties are expected to be most pronounced. Here, I will present our discovery of all-inorganic helical crystals which display highly tunable tetrahelical motifs based on the distinct and modular class of III-VI-VII 1D van der Waals (vdW) crystals. I will discuss how a series of structural and spectroscopic characterization techniques led to the realization of atypical helical geometries, non-linear optical properties, and highly resolved temperature-sensitive optical signatures. Examples that I will describe include our first demonstration of the rare aperiodic/quasi-crystalline inorganic Boerdijk-Coxeter helix motif in GaSeI,¹ the chalcogen substitution-induced “squircular” motif in GaSI,² and the highly temperature absorption edges in the visible range thermochromic InSeI phase.³ I will conclude by briefly describing our recent advances in understanding the bottom-up growth pathways of 1D vdW helices into ultra-thin (sub-10 nm-thick) nanowires, their non-optical properties, and potential for spin-polarized behavior. The centrality of helicity in a multitude of nascent physical phenomena makes this class of inorganic 1D vdW helices a suitable platform to systematically probe the complex physics and device applications that emerge from dense solid-state helical structures.

Keywords: helical crystals, structural chirality, 1D van der Waals solids, nanowires, second-harmonic generation, chiral-induced spin selectivity

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EXCEPTIONALLY STABLE METATHESIS CATALYSTS FOR GREEN CHEMISTRY

Bartosz Trzaskowski^{a,*}

^aCentre of New Technologies, University of Warsaw

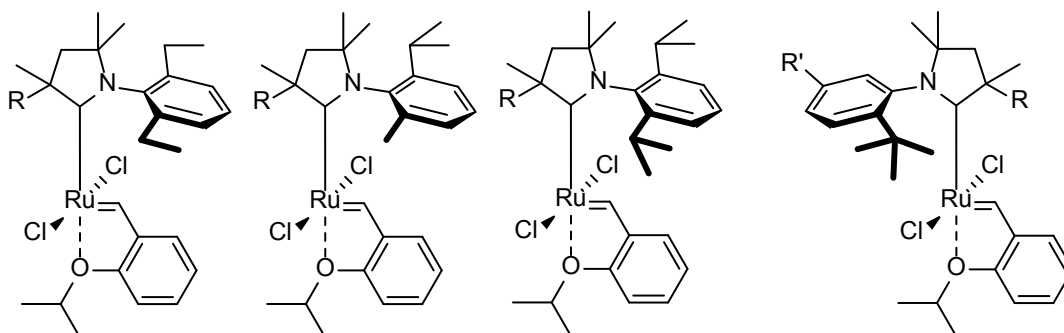
*Corresponding author: b.trzaskowski@cent.uw.edu.pl

Abstract

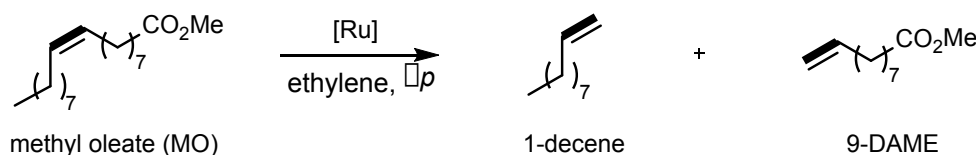
The olefin metathesis reaction of forming new C-C bonds is one of the most important reactions in organic synthesis. We have developed ruthenium-based Hoveyda-type olefin metathesis catalysts bearing novel rigid spirocyclic alkyl amino carbenes (CAACs), which are characterized by exceptional stability toward decomposition through β -elimination and bimolecular pathways, thus enabling unprecedented efficiency in the cross-metathesis of seed oil-derived fatty acid esters with ethylene (ethenolysis).¹ Using a catalyst concentration as low as 100 parts per billion, the ethenolysis of methyl oleate, a model substrate, achieved an extraordinary turnover number (TON) of 2.6 million. This result surpasses previous records, which demonstrated TONs of 340,000 at 1 ppm and 744,000 at 0.5 ppm catalyst loading. For the first time, a highly efficient ethenolysis process was demonstrated using readily accessible and cost-effective renewable resources: methyl esters from high oleic sunflower oil and rapeseed oil. This breakthrough achieved an impressive turnover number (TON) of 964,000 with a remarkably low catalyst loading of 0.5 ppm. We also showed how simple computational parameters are able to quickly predict efficiency of metathesis catalysts.²

Keywords: olefin metathesis, catalysis, green chemistry, modelling, decomposition

[Ru] catalysts



catalyzed reaction



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DI-(2-PICOLYL)AMINE DERIVATIZED SULFONAMIDE LIGANDS AND PLATINUM COMPLEXES FOR PROSPECTIVE BIOIMAGING APPLICATIONS

Kithmini Yasarathna^{a,b}, Praneeth Rathnayake^c, Inoka Perera^c, Theshini Perera^{a,*}

^aDepartment of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda, Sri Lanka.

^bDepartment of Pharmacy, Faculty of Allied Health Sciences, University of Ruhuna, Galle, Sri Lanka.

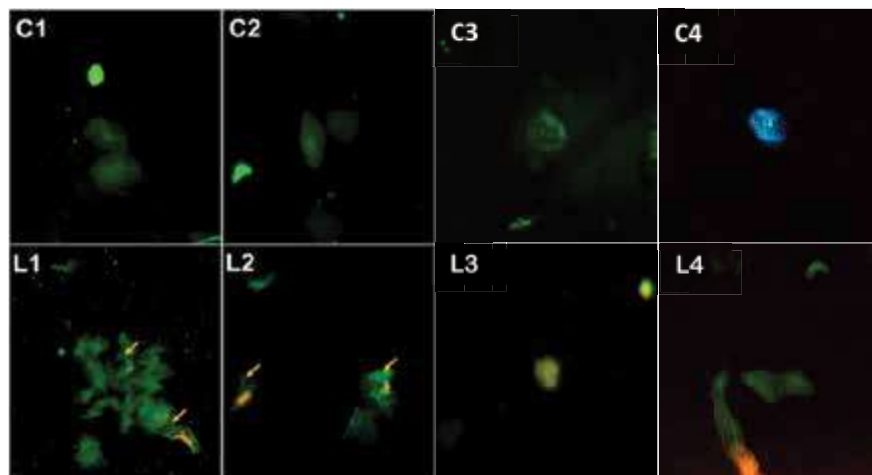
^cDepartment of Zoology and Environment Sciences, University of Colombo, Colombo 03, Sri Lanka.

*Corresponding author: theshi@sjp.ac.lk

Abstract

Many transition metal-based complexes of Pt(II), Re(I) and gamma emitting ^{99m}Tc have been used as bioimaging agents, as they possess important biomedical properties including photo-physical properties and radioactivity.¹ With the intention of identifying novel drug leads with potential bioimaging properties, four di-(2-picoly)amine derivatized sulfonamide ligands; N(SO₂tmb)dpa (L1), N(SO₂chlorobenzene)dpa (L2), N(SO₂pyr)dpa (L3) and N(SO₂Meimid)dpa (L4) and their corresponding platinum complexes; [Pt(N(SO₂tmb)dpa)Cl₂] (C1), [Pt(N(SO₂chlorobenzene)dpa)Cl₂] (C2), Pt(N(SO₂pyr)dpa)Cl₂ (C3) and Pt(N(SO₂Meimid)dpa)Cl₂ (C4) were synthesized. After successful characterization, fluorescence spectroscopy was conducted for preliminary observation of the imaging applicability of the synthesized compounds. Possible biological application of these ligands and complexes as bioimaging agents were evaluated through fluorescent microscopy. Isolated human buccal epithelial cells were treated with each ligand and complex, incubated for 8 min at room temperature and cells were observed with fluorescent microscope. Ligands displayed high fluorescence intensities while quenched fluorescence was observed in Pt complexes. When the incubated buccal epithelial cells were observed under the fluorescence microscope, enhanced fluorescence was observed inside the cells. Fluorescence images taken for the ligands; L1 – L4 and complexes; C1 – C4 showed accumulation of these compounds that led to increase the fluorescence inside the cells. These images confirm the successful cellular uptake of all the compounds. Any morphological changes or cytotoxic effects in buccal epithelial cells were not observed after incubation with the tested compounds. These sulfonamide ligands and their platinum complexes can be identified as effective fluorophores for the tested cell type and thus, can be further investigated as potential bioimaging agents.

Keywords: bioimaging, di-(2-picoly)amine, fluorescence, platinum complexes, sulfonamide ligands



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SYNTHESIS AND INVESTIGATION OF CHEMOMECHANICAL GELS DRIVEN BY THE BELOUSOV-ZHABOTINSKY REACTION: INSIGHTS INTO LIGAND INFLUENCE

Olga V. Lagunova^{a,*}, Pavel S. Smelov^a, Ilya L. Mallphanov^a, Alexander V. Sychev^b, Eugeny G. Chupakhin^a

^a*Center for Applied Nonlinear Dynamics, Immanuel Kant Baltic Federal University, Russia.*

^b*Research Center for Condensed Matter Physics, Kursk State University, Russia.*

*propagalagunova@gmail.com

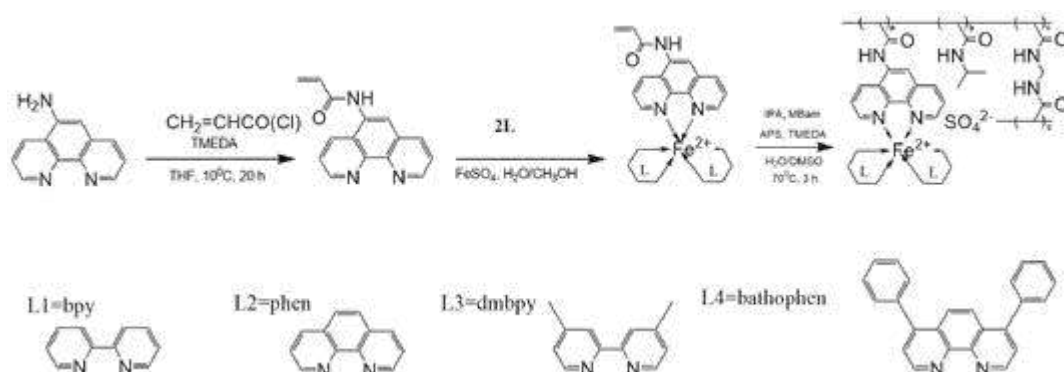
Abstract

The synthesis and study of a novel class of “smart” materials — self-oscillating chemomechanical gels activated by the Belousov-Zhabotinsky (BZ) reaction — are gaining significant attention globally due to their potential applications in innovative systems such as actuators, liquid transport devices, and chemical signal processors^{1,2}. Despite notable advancements in this field, critical challenges remain unresolved, particularly the absence of a unified theory that elucidates how the nature of ligands in metal complex catalysts affects the amplitude of the chemomechanical response in these gels.

We have synthesized heteroleptic complex compounds with catalytic activity in the BZ reaction: Fe(phen)₂(acphen), Fe(dmbpy)₂(acphen), and Fe(bpy)₂(acphen), and also Fe(bathophen)₂(acphen)³, which incorporate acrylamide fragments within the phenanthroline ligand. Isopropylacrylamide-based gels containing immobilized synthesized BZ catalysts were prepared and characterized in terms of their morphological and spectral properties. The autocatalytic behavior of the resulting hydrogels during the BZ reaction was investigated. The study revealed that as the hydrophobicity of the ligand increases, so does the amplitude of the chemomechanical oscillations, highlighting a significant relationship between ligand characteristics and gel responsiveness. These findings pave the way for further exploration into optimizing ligand design to enhance the performance of chemomechanical gels in various applications, addressing existing challenges in the field.

This research was supported by funds provided through the Russian Federal Academic Leadership Program “Priority 2030” at the Immanuel Kant Baltic Federal University, project number 124021400010-7

Keywords: iron complexes, smart materials, self-oscillating gels, Belousov-Zhabotinsky reaction.



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METAL COMPLEXES AT THE BINDING SITES OF BACTERIAL VIRULENCE FACTORS

Anna Rola^a, Paulina Potok^a, Martyna Zawada^a, Elżbieta Gumienna-Kontecka^a, Sławomir Potocki^{a*}

^a Faculty of Chemistry, University of Wrocław, 14 Joliot-Curie St., 50-383, Wrocław, Poland

*Corresponding author: slawomir.potocki@uw.edu.pl

Abstract

The rising prevalence of antibiotic-resistant pathogens has become a major global health challenge, driving the search for new therapeutic protein targets in bacteria. Here we present results on metal complexes of important metal-dependent virulence factors binding sites and the influence of point mutations on their thermodynamic properties. We have studied SmtB/BigR4 transcriptional regulators (*M. tuberculosis*/*M. smegmatis*) [1, 2], GroEL1 chaperonins (mycobacteria) [3, 4], and metallopeptidases (e.g. *S. pneumonia*) [5].

The thermodynamic properties of M(II) complexes (including Zn, Ni, and Cu) were investigated using potentiometry, NMR, MS, UV-Vis, CD, EPR, and DFT methods. Introducing targeted mutations enabled the identification of key side chains essential for binding biologically relevant metals. Our research aims to pinpoint critical alterations in the protein sequence that could be crucial for designing drugs targeting these molecular structures. Additionally, it contributes to a deeper understanding of metal interactions with key virulence factors, which play a vital role in pathogen homeostasis.



Examples of virulence factors (from left): chaperonin GroEL1,⁴ metallopeptidase M10 (UniProt - A0A2U3RYI4), transcriptional regulator SmtB (PDB - 8QKF).

Keywords: virulence factors, bacteria, metal complexes, binding sites, thermodynamics

Acknowledgements

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A YOLK@SHELL NANOARCHITECTURE FOR NIMN@AL₂O₃ CATALYSTS

Asikin-Mijan^{a,*}, AbdulKareem-Alsultan^b, OthamanNAA^a, SulaimanM^a, Nur Athirah Adzahar^{a,b}

^aDepartment of Chemical Sciences, Faculty of Science and Technology, Universiti

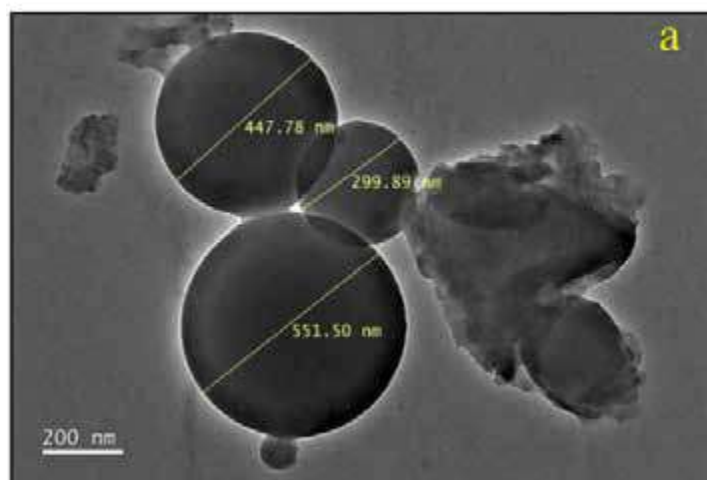
^bCatalysis Science and Technology Research Centre, Faculty of Science, Universiti Putra Malaysia, 43400 UPM
Serdang, Selangor, Malaysia

*Corresponding author: nurul.asikin@ukm.edu.my

Abstract

Eco-friendly and cost-effective catalysts are gaining significant interest for commercialization, particularly in oil and gas processing reactions. In this study, a yolk-shell catalyst was synthesized using nickel, manganese, and Al₂O₃. The core-shell catalysts were thoroughly characterized using XRD, BET, TPD-NH₃, and HRTEM. Additionally, the surface properties of the metals were examined using Scanning Tunneling Microscopy (STM), a powerful technique for visualizing materials at the atomic and molecular scale. This study provides a detailed mechanistic insight into the development and properties of the core-shell structure. Preliminary investigations on oil and gas processing using the yolk-shell catalyst are also discussed, highlighting its role in enhancing catalytic performance.

Keywords: Catalyst, nickel, manganese, nanocatalyst, yolk-shell



HRTEM of core shell catalyst.

MIXED-POTENTIAL-DRIVEN CATALYSIS: AN ELECTROCHEMICAL MECHANISM FOR ROOM-TEMPERATURE CO OXIDATION ON GOLD CATALYSTS

Mo Yan^a, Asif Muhammad^b, Ravi Singh^b, Kotaro Takeyasu^{c,d}, and Junji Nakamura^{a,*}

^aInternational Institute for Carbon-Neutral Energy Research (FCNER), Kyushu University; 744 Motoooka, Nishi-ku, Fukuoka-shi, Fukuoka 819-0395, Japan.

^bGraduate School of Science and Technology, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan.

^cInstitute of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan.

^dInstitute for Catalysis, Hokkaido University, Kita21, Nishi10, Kita-ku, Sapporo, Hokkaido 001-0021, Japan

*Corresponding author: nakamura.junji.700@m.kyushu-u.ac.jp

Abstract

Gold is a highly effective catalyst for the low-temperature oxidation of CO to CO₂ ($\text{CO} + 1/2 \text{O}_2 \rightarrow \text{CO}_2$), yet ongoing studies continue to debate the crucial characteristics of this catalyst.¹ Recently, there has been a growing appreciation that thermochemical catalysis involving water actually proceeds via two coupled electrochemical half-reactions.² Here, we report the experimental evidence that the room-temperature CO oxidation with water could proceed via coupled electrochemical CO oxidation and oxygen reduction half-reactions, i.e., the mixed-potential-driven mechanism. A model system was designed with deposited Au nanoparticles and nitrogen-doped reduced graphene oxide on carbon paper acting as spatially separated electrodes in a single electrolysis cell. After shorting the two electrodes, the reaction current and mixed potential were measured without any bias potential. Independent current–potential curves for each half-reaction under identical conditions were obtained, and the predicted mixed potential and mixed current were compared with that measured by the model system, showing good agreement. Therefore, it was shown that the driving force of CO oxidation is used to accelerate the half-reactions at low temperatures, and water plays the role of an electrolyte solvent. This study provides a definitive answer to the controversy regarding the mechanism of the Au-catalyzed CO oxidation.

Keywords: mixed potential, CO oxidation, heterogenous catalysis, electrochemical half-reaction, reaction pathway

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HIGH-PERFORMANCE NANOZYMES: RATIONAL DESIGN AND BIOMEDICAL APPLICATIONS

Hui Wei^{a,b,c*}

^aDepartment of Biomedical Engineering, College of Engineering and Applied Sciences, Nanjing University, Nanjing, Jiangsu 210023, China.

^b Nanozyme Laboratory in Zhongyuan, Henan Academy of Innovations in Medical Science, Zhengzhou, Henan 451163, P. R. China.

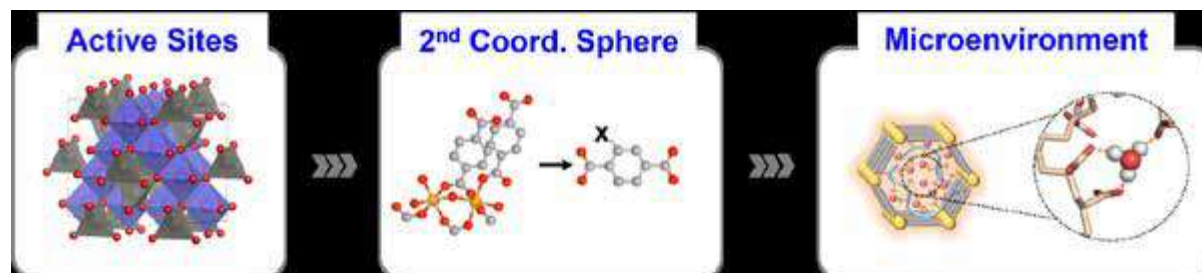
^cState Key Laboratory of Analytical Chemistry for Life Science, Chemistry and Biomedicine Innovation Center (ChemBIC), Nanjing University, Nanjing, Jiangsu 210023, China.

*Corresponding author: weihui@nju.edu.cn

Abstract

Nanozymes are functional nanomaterials with enzyme-like activities. They are superior to natural enzymes and conventional enzyme mimics in several aspects, including high stability, enduring catalysis, tunable activity, facile engineering, etc. The design of high-performance nanozymes is challenging because of the complicated structures and ambiguous active sites. To this end, we developed several cross-material design rules for guiding the design of high-performance nanozymes. Specifically, we were able to design and tune the active sites, 2nd coordination sphere, and microenvironment of nanozymes, achieving 1-2 orders of magnitude higher activity compared with the reported nanozymes. We further explore their biomedical applications, particularly focused on reactive oxygen species-related diseases. Our studies demonstrate the promise of nanozymes for precision medicine.

Keywords: nanozymes, enzyme mimics, functional nanomaterials, rational design



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SOLAR HYDROGEN PRODUCTION UNDER THE CARIBBEAN SUN

Jorge L. Colón ^{a*}

^a*University of Puerto Rico, Río Piedras.*

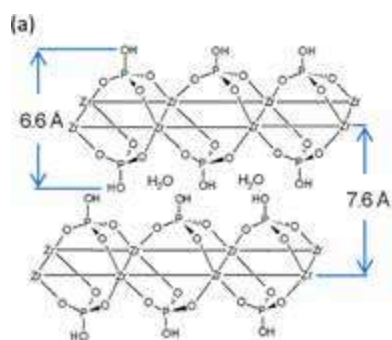
**Corresponding author: jorge.colon10@upr.edu*

Abstract

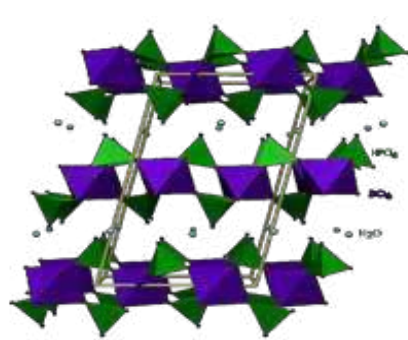
Our work is focused on the use of layered zirconium phosphate (ZrP) nanomaterials as supports for photo- and electrocatalysts for hydrogen production via water splitting.¹ The theta phase of ZrP ($\text{Zr}(\text{HPO}_4)_2 \cdot 6\text{H}_2\text{O}$, θ -ZrP) can be directly ion-exchanged with metal complexes and catalysts, producing intercalated phases useful for water splitting applications. Studies of transition metal oxides as earth-abundant and non-precious catalysts have increased in recent years. Recently, we have demonstrated improved electrocatalytic activity of layered ZrP nanomaterials loaded with earth-abundant Co^{2+} , Ni^{2+} , or Fe^{2+} metal ions suitable as catalysts for the oxygen evolution reaction (OER) of water splitting. Electrocatalysts have been adsorbed on the external surface of ZrP nanoparticles, or incorporated as intercalated species, or adsorbed on individual exfoliated layers, and adsorbed on nanoparticles with different morphologies (hexagonal platelets, cubes, rods, and spheres). Single and bimetallic electrocatalysts based on these earth-abundant metals have been studied. Reduction in overpotentials and increases in mass activity have been achieved. Mixed metal NiFe-intercalated ZrP electrocatalysts at 90% Fe metal content proved to have superior OER electrocatalytic performance (decreased overpotentials, increased mass activities, reduced Tafel slopes) compared to adsorbed counterparts. Recently, we have prepared CoFe-based electrocatalyst systems adsorbed on the external surface of $\text{Zr}(\text{HPO}_4)_2 \cdot \text{H}_2\text{O}$ (α -ZrP) nanoparticles or intercalated between the ZrP layers using θ -ZrP. The CoFe intercalated system is more active (lower overpotential) than the surface adsorbed one, consistent with the NiFe results. We are studying the OER activities of other mixed-metal catalysts (including Mn-based ones) and if they can be bifunctional catalysts (OER and ORR or HER activity), and conducting *operando* synchrotron XAS studies to elucidate the nature of the electrocatalytic active species. We are also exploring efficient solar H_2 production using these supports by incorporating photoadsorbers in photoelectrochemical cells.

Keywords: Zirconium phosphate, nanomaterials, water splitting, electrocatalysis

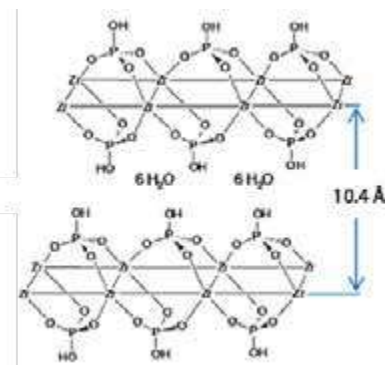
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(a) Idealized structure of α -ZrP



(b) Polyhedral structure of α -ZrP



(c) Idealized structure of α -ZrP

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RUTHENIUM AND RHENIUM-BASED PHOTOSENSITIZERS: ADVANCING PHOTODYNAMIC THERAPY FOR ANTICANCER AND ANTIBACTERIAL APPLICATIONS

May Lee Low^{a,*}, Xiao Ying Ng^b, Kar Wai Fong^b, Hui Shan Liew^b, Kuan Teng Tan^a

^a Faculty of Pharmaceutical Sciences, UCSI University, Malaysia.

^b School of Postgraduate Studies, IMU University, Malaysia.

*Corresponding author: lowml@ucsiuniversity.edu.my

Abstract

Photodynamic therapy (PDT) has emerged as a promising approach for cancer treatment and combating multidrug-resistant (MDR) bacterial infections. This technique relies on photosensitizers that, upon light activation, generate reactive oxygen species to induce targeted cell death. Transition metal-based photosensitizers, particularly ruthenium(II) and rhenium(I) complexes, have gained attention due to their tunable ligand architectures, efficient singlet oxygen generation, and redox-active excited states, enabling precise light-activated cytotoxicity. In this study, Ru(II) polypyridyl and Re(I) tricarbonyl complexes were synthesised and structurally optimised for enhanced biological targeting. To improve solubility and selectivity, the complexes were conjugated with targeting agents and encapsulated into liquid crystalline nanoparticles (LCNPs), which enhanced stability and cellular uptake. The compounds were evaluated across multiple cancer cell lines and MDR bacterial strains to determine their therapeutic potential. Our findings also highlight these metal-based photosensitizers as promising adjunct therapies, particularly in combination with conventional agents. The enhanced biological activities further support their integration into targeted anticancer and antibacterial strategies. The combination of strategic ligand design and nanocarrier delivery improves therapeutic efficacy, offering a viable translational approach for treating resistant cancers and bacterial infections. This study underscores the versatility of Ru and Re metal complexes in photomedicine, paving the way for advancements in PDT-based combination therapies.

Keywords: Photodynamic therapy, ruthenium complexes, rhenium complexes, anticancer, antibacterial

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EFFECT OF SUSTAINABLY DERIVED 45S5 BIOGLASS ON THE PROPERTIES OF BIOWASTE-DERIVED HYDROXYAPATITE COMPOSITES

S.L.Tan^a, C.K. Ng^{a,*}, T.K. Ong^a, C.H. Ting^b, W. H. Yeo^b, S. Ramesh^c

^a Centre for Advanced Materials, Department of Manufacturing Technology, Faculty of Engineering & Technology, Tunku Abdul Rahman University of Management and Technology, 53300, Kuala Lumpur, Malaysia

^b Department of Mechanical and Materials & Manufacturing Engineering, Lee Kong Chian Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, Jalan Sungai Long, Bandar Sungai Long, Cheras, Kajang 43000, Malaysia

^c Centre of Advanced Manufacturing and Material Processing, Department of Mechanical Engineering, Faculty of Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia

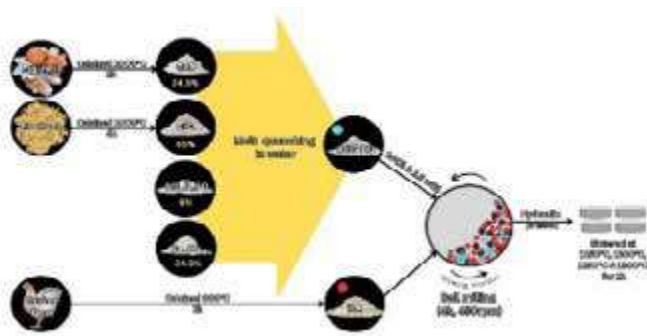
*Corresponding author: ngck@taru.edu.my (C.K. Ng).

Abstract

Hydroxyapatite (HA) is widely recognized as a bioceramic due to its chemical similarity to the inorganic components of bone and teeth. However, a drawback of HA as an implant, when compared to bioactive glasses and other ceramics is its relatively low reactivity with natural bone, which slows the process of bone attachment and integration [1]. Previous studies have shown that incorporation of small amounts of bioglass (BG) enhances the flexural strength and fracture toughness of mechanically reinforced bioactive composites [2]. To address this, 45S5 bioglass (BG) derived from sustainable sources (eggshells for CaO and rice husk for SiO₂) was incorporated into HA synthesized from chicken bones. This study investigates the effects of 1 wt% and 2.5 wt% BG additions on the mechanical properties of HA composites sintered at 1150–1300°C. HA-BG powders were homogenized via ball milling, compacted, and subjected to cold isostatic pressing. X-ray diffraction revealed minor HA decomposition into β -tricalcium phosphate (β -TCP), indicating non-stoichiometric phase formation. The composite with 1 wt% BG sintered at 1200°C exhibited optimal properties, achieving a relative density >95%, a fracture toughness of 1.36 MPa·m^{1/2}, and a hardness of 4.99 GPa. Additionally, fracture toughness was found to stabilise at higher sintering temperatures. In conclusion, the effect of BG on HA varied, with mechanical properties improving or deteriorating depending on the BG content and sintering conditions. These findings highlight the potential of sustainable HA-BG composites in orthopedic engineering, dependent on BG content and sintering temperature.

Keywords: Biowaste; Hydroxyapatite; Bioglass

Graphic / Image



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MULTIPATH LUMINESCENCE OF METAL-ORGANIC COMPLEXES

Mei Pan*

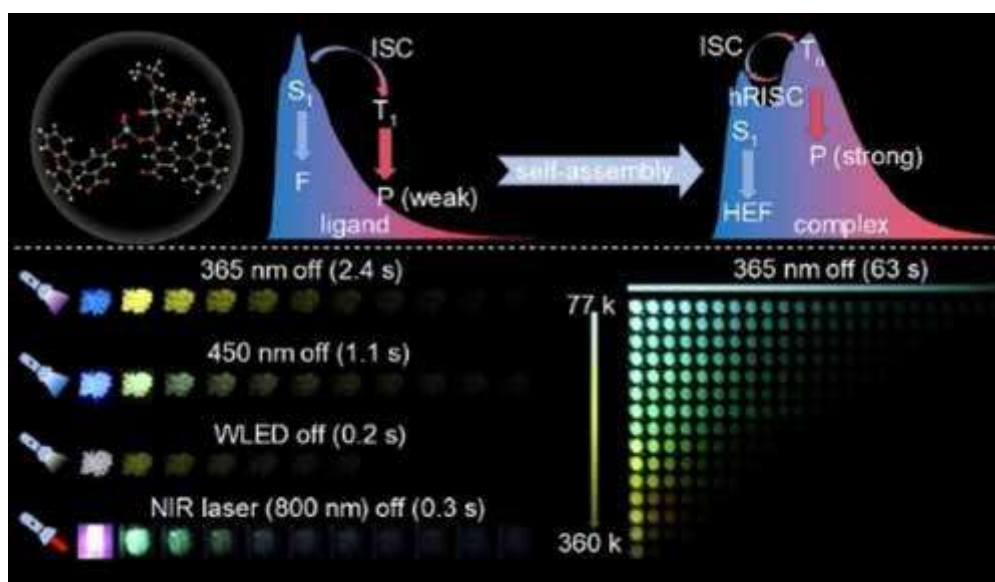
School of Chemistry, Sun Yat-Sen University, Guangzhou, 510006

**Corresponding author: panm@mail.sysu.edu.cn*

Abstract

Metal-organic complexes have emerged as a research hotspot in chemistry and materials science due to their unique structures and multifunctional characteristics. These compounds not only combine the advantages of organic and inorganic components, but also exhibit abundant luminescent properties, offering the possibility of achieving multipath luminescence and modulation. In recent years, our group has focused on the structural design and optical performance regulation of metal-organic complex materials, and obtained novel and highly efficient metal-organic photofunctional materials with multipath excitation long afterglow, temperature-responsive luminescence, and acid-base-responsive luminescence, respectively.

Keywords: metal-organic complexes, long afterglow, stimuli-responsive luminescence



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DEVELOPMENT OF NEW RECYCLABLE CATALYSTS FOR SIMPLE ORGANIC TRANSFORMATIONS

Muhammad Dabai Bala^{a,*}

^a*School of Chemistry and Physics, University of KwaZulu-Natal, Durban, South Africa*

^{*}*Corresponding author: bala@ukzn.ac.za*

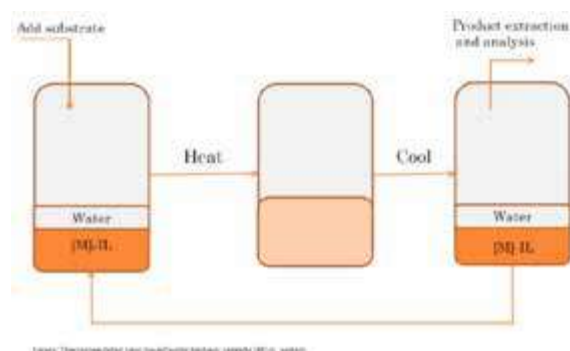
Abstract

Recyclable homogeneous catalysis offers the advantages of both homogeneous and heterogeneous catalysis while limiting the shortcomings of each; hence, it is a long-cherished goal of chemists in academia and industry. We have developed novel transition metal complexes as highly active homogeneous catalysts for various applications.¹ Herein, we will discuss some of our attempts at improving the sustainability credentials of the catalysts by focusing on the following:

1. Triazolium ionic liquids (ILs) were synthesized using the facile and atom economic azide-alkyne ‘click’ cycloaddition reaction. With the ILs as solvents for the dissolution of metal salts {[M] = FeCl₂, FeCl₃, CoCl₂, and NiCl₂ (Fig)}, a series of catalyst systems were developed and used to activate the catalytic oxidation of n-octane in a biphasic IL/H₂O system. All systems tested were found to be recyclable and active under optimum conditions, yielding oxygenated C-8 products.²
2. A new methodology was developed for immobilizing triazolium salts onto polyethylene glycols (PEGs) to produce polymer ionic liquids (PILs). The PILs were fully characterized and utilized as recyclable metal-free organocatalysts for the H₂-free transfer of hydrogenation of ketones to alcohols in isopropanol as solvent and hydrogen source. The metal-free PIL catalysts showed activity for transforming acetophenone to 1-phenyl alcohol at up to 87% conversion.³

In conclusion, we have illustrated examples of modifying homogeneous catalysts for recyclability and sustainability, a key pillar of the UN Millennium Development Goals.

Keywords: Ionic liquids; Thermoregulated catalysis; Oxidation; Transfer hydrogenation.



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BIGUANIDE METAL COMPLEXES AS EFFICIENT ROP CATALYSTS FOR SUSTAINABLE (CO-)POLYMERS

Lukas Vlk^{a,*}, Tomas Chlupaty^a, Benjamin Theron^b, Damien Breilly^b, Zdenka Ruzickova^a, Raluca Malacea-Kabbara^b, Pierre Le Gendre^b, Ales Ruzicka^a

^a Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentska, 573, 53210 Pardubice, Czech Republic.

^b Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB, UMR-CNRS 6302), University of Burgundy, 9 Avenue Alain Savary, 21000 Dijon, France.

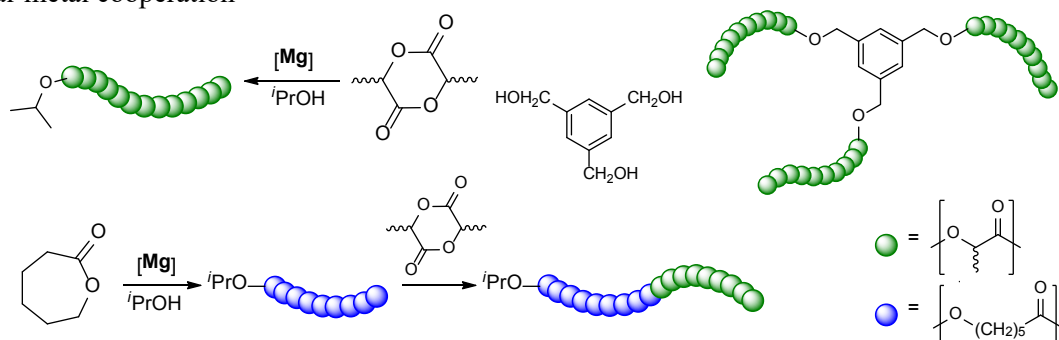
*Corresponding author: st54138@upce.cz

Abstract

One of the biggest drawbacks in modern polymer chemistry is the heavy impact of current petrol-based plastics on the environment both in terms of origin and the after-use waste processing. Hence, efforts to replace these materials with bio-degradable polymers are underway, with the family of cyclic esters – most prominently lactide available from renewable natural sources – emerging as a viable alternative.¹ However, by far the most common industrial catalyst for ring-opening polymerization (ROP) of lactide to polylactic acid (PLA) is tin octoate, which has been determined as toxic. A suitable replacement has not been yet introduced, although several transition or main group metal compounds (oxides, alkoxides and a plethora of complexes) were used for ROP of lactide in recent years. One of the most active systems employed an *N*-donor multidentate ligands stabilizing metal amides.²

Our research in recent years has developed a capable ligand platform for controlled structural arrangement of multimetallic guanidinate/biguanide complexes. The first trial tests showed promising activity and control of some compounds in ROP of lactide. After pursuing this route, we were able to tailor exceptional Mg and Zn-based catalysts for ROP of cyclic esters, demonstrated on monomers like lactide, ϵ -caprolactone, β -butyrolactone and trimethylenecarbonate. The highly active and robust species were able to polymerize several thousand equivalents of the monomer in minutes at room temperature. The most efficient catalysts surpassed turn-over frequencies of 60 000 h⁻¹ in lactide ROP. Moreover, di- and triblock co-polymers of some combinations of *rac*-, *L*-, *D*-lactide, ϵ -caprolactone and β -butyrolactone were obtained in immortal catalytic conditions, showcasing the power of a truly universal, active and immortal catalyst.

Keywords: biguanide metal complexes, ROP catalysis, sustainable (co-)polymers, main group metal catalysis, tunable metal-metal cooperation



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DESIGN OF MULTICOLOR SOLID-STATE FLUORESCENCE AND GREEN PHOSPHORESCENCE OF PHENYLENEDIAMINE-BASED CARBON DOTS

Pinyi He^a, Jianliang Bai^a, Guohui Yang^a, Fu Qin^a, Lili Ren^{a,*}

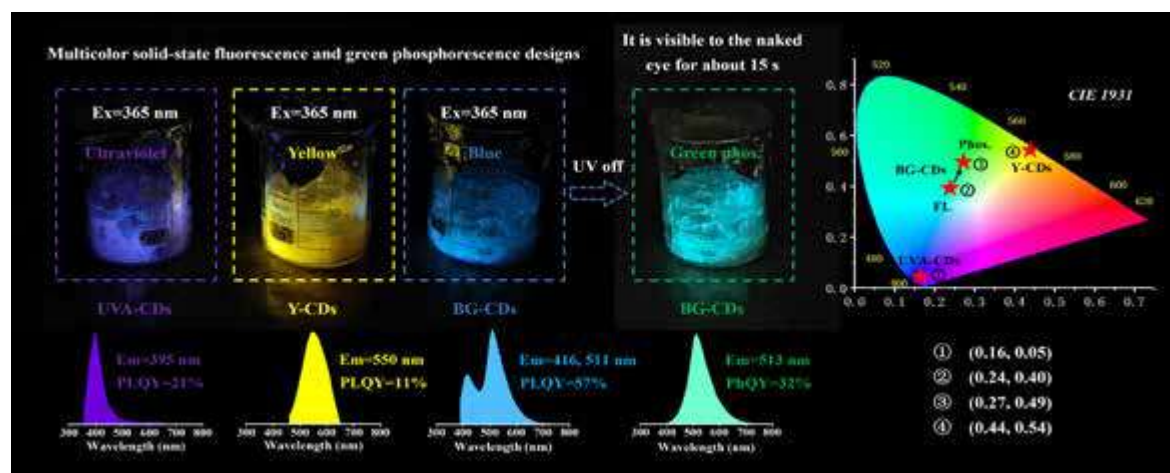
^a*School of Chemistry & Chemical Engineering, Southeast University*

**Corresponding author: liliren@seu.edu.cn*

Abstract

Carbon dots (CDs) are a kind of fluorescent nanoparticles with environmentally friendly, excellent optical performance, and simple preparation methods. At present, phenylenediamine (PD) has become a classic material for synthesizing CDs due to its nitrogen doping and conjugated structure. Many studies focused on the fluorescence regulation of PD-based CDs to realize colorful displays. Our group also designed multicolor solution-state fluorescence of PD-based CDs in these years.¹⁻³ However, due to the aggregation-induced quenching effect and non-radiative transitions of triplet excitons, multicolor solid-state CDs are difficult to achieve, which greatly limits their application and development in lighting and advanced anti-counterfeiting. Based on this, we used PD as the raw material and adopted a synergistic fixation and dispersion strategy with rigid matrix and silane agent to achieve a design of solid-state ultraviolet A emissive CDs (395 nm), yellow CDs (550 nm), and green phosphorescent CDs (513 nm). The optical properties and structure analysis prove that the quantum size effect, sp²-conjugated domain, and graphite N content determine solid-state fluorescence colors. In addition, we also elucidated the reasons for achieving green phosphorescence activation. Finally, different fluorescent colors and green phosphorescence properties are utilized to achieve advanced encryption and anti-counterfeiting applications. This work will pave the way for multicolor fluorescent and phosphorescent designs of solid-state CDs.

Keywords: phenylenediamine, carbon dots, solid-state fluorescence, phosphorescence



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NI–LA PEROVSKITES FOR EFFICIENT CO₂ VALORIZATION AND INDOOR AIR QUALITY IMPROVEMENT

Luca Consentino^{a,b,*}, Miriam González-Castaño^c, Nuría Garcia-Moncada^d, Luis F. Bobadilla^c,
Michelangelo Gruttadauria^b, Leonarda Francesca Liotta^a, José Antonio Odriozola^{c,e}

^a ISMN-CNR, Via U. La Malfa 153, 900146 Palermo, Italy

^b STEBICEF Department Ed. 17, University of Palermo, Viale delle Scienze, 90128 Palermo, Italy

^c Department of Inorganic Chemistry, University of Seville (ICMS-CSIC), C/Americo Vespucio 49, 41092 Seville, Spain

^d General Research Services, XPS, Research, Technology, and Innovation Center of the University of Seville (CITIUS), Av. Reina Mercedes 4B, 41012 Seville, Spain

^e College of Environmental Science and Engineering, Beijing Forestry University, 35 Qinghua East Road, Haidian District, Beijing 100083, P. R. China

*Corresponding author: lucaconsentino@cnr.it

Abstract

The transition toward a low-carbon energy system calls for innovative solutions capable of closing the carbon cycle and storing renewable energy¹. In parallel, the accumulation of carbon dioxide in indoor environments—especially in sealed or energy-efficient buildings—poses a growing concern for indoor air quality (IAQ) and health. Among emerging strategies, the catalytic methanation of CO₂ represents a key process for converting captured carbon dioxide into synthetic natural gas (SNG), facilitating both energy storage, carbon reuse, and potentially, reactive indoor CO₂ abatement. When integrated into IAQ management systems, methanation offers a dual opportunity to remove indoor CO₂ while generating on-site energy, as in micro-CHP applications. This reaction is based on the Sabatier reaction ($\text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{H}_2\text{O}$) a thermodynamically favourable process that faces kinetic limitations and demands highly active catalysts to achieve efficient conversion. In this work, Ni–La perovskite-based catalysts were investigated with particular focus on their structural dynamics and redox behavior². Catalysts were synthesized via microwave-assisted method³ using two approaches: a one-pot synthesis (MW-OP) and an impregnation route (MW-Imp). The study aimed to elucidate how Ni incorporation strategy and reduction temperature influence key structural features—such as Ni dispersion, oxygen vacancy density, and metal–support interactions—that influence catalytic performance. Samples reduced at 500 °C and 750 °C were compared to assess the impact of thermal treatment on phase evolution and activity. Multiple complementary techniques, including XRD, H₂-TPR, NAP-XPS, and in situ DRIFTS-MS, were used to investigate the structural, redox, and surface properties of the catalysts. The results underscore the influence of synthesis route and reduction conditions on the generation of active sites and surface species involved in CO₂ activation. The comparison between MW-OP and MW-Imp samples demonstrates that structural modifications significantly affect CO₂ conversion, methane yield, and catalyst stability. These findings contribute to a deeper understanding of structure–function relationships in Ni-based perovskite systems and support the rational design of efficient catalytic materials for CO₂ abatement and valorization, with relevance to power-to-gas technologies, carbon reuse strategies and IAQ improvement.

Keywords: CO₂ abatement and valorization, Ni–La perovskite, catalysts structure, energy transition, IAQ control.

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STRUCTURAL DIVERSITY OF LANTHANIDE COMPLEXES FUNCTIONAL TO THEIR SEPARATION AND RECOVERY

Luciano Marchiò^{a,*}, Matteo Melegari^a, Angela Serpe^{b,c}, Alex Falco^a, Matteo Tegoni^a.

^aDepartment of Chemistry, Life Sciences and Environmental Sustainability, University of Parma, Italy.

^bDepartment of Civil and Environmental Engineering and Architecture, University of Cagliari, Italy.

^cEnvironmental Geology and Geoengineering Institute of the National Research Council, Cagliari, Italy.

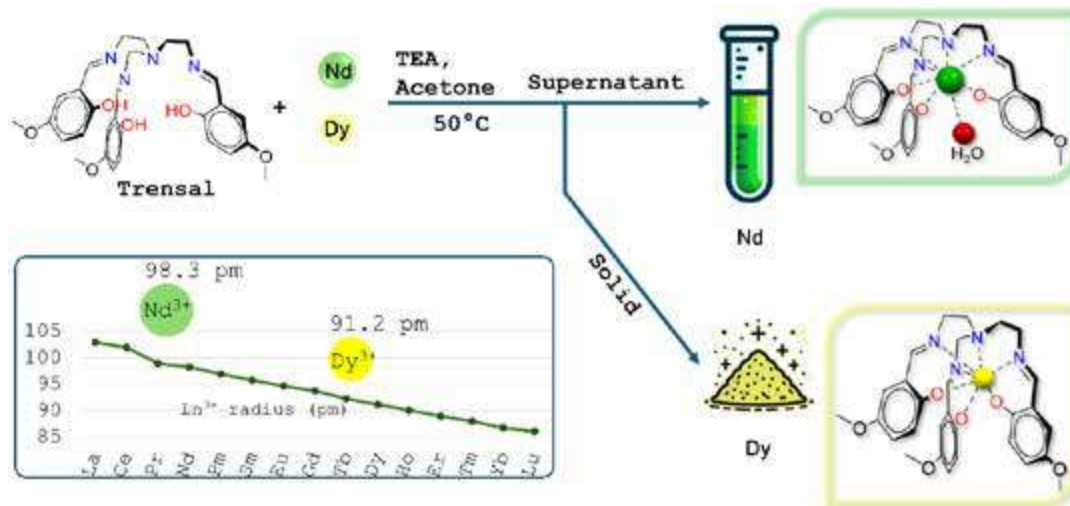
*Corresponding author: luciano.marchio@unipr.it

Abstract

Rare Earth Elements (REEs), which include the lanthanides plus scandium and yttrium, are indispensable for the operation of high-tech products due to their unique optical and magnetic properties. However, in recent years, the escalating demand for these critical technological metals has far exceeded their availability¹. Traditional methods for recycling these elements have struggled to keep pace, capturing only 5% of industry demand, largely due to the prohibitive costs and significant environmental challenges associated with these processes².

Our study specifically addresses the selective separation and recovery of metals used in high-performance NdFeB magnets, which are widespread in electronic devices, wind turbines, rechargeable batteries, and electric vehicles. These magnets typically consist of iron (65%), neodymium (Nd, 25-30%), and dysprosium (Dy, 1-3%). For the separation studies, we have employed N4O3 polydentate ligands that are suitable for the coordination of lanthanide cations. However, while Nd³⁺ and Dy³⁺ have very similar chemical characteristics, they have substantial differences (such as ionic radius and coordination number) that allow ligands to be designed that satisfy the stereoelectronic requirements of one metal over the other^{3,4}. Hence, Nd³⁺ and Dy³⁺ complexes show different solubility in organic solvents based on the subtle chemical differences between the two metals, which is relevant for the separation of REE cations.

Keywords: Rare-earth elements, Dysprosium and Neodymium complexation, Selective precipitation for metal recovery.



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BRANCHED-CATION-INCORPORATED TWO-DIMENSIONAL PEROVSKITES: STRUCTURAL EVOLUTION AND OPTOELECTRONIC APPLICATIONS

Wenxuan Li^a, Jianjia He^a, Yilan Zhang^a, Guoying Yao^a, Tao Zeng^b, Zhenyu Yang^{a,*}

^aMOE Laboratory of Bioinorganic and Synthetic Chemistry, Lehn Institute of Functional Materials, School of Chemistry, Sun Yat-sen University, Guangzhou 510275, Guangdong, China

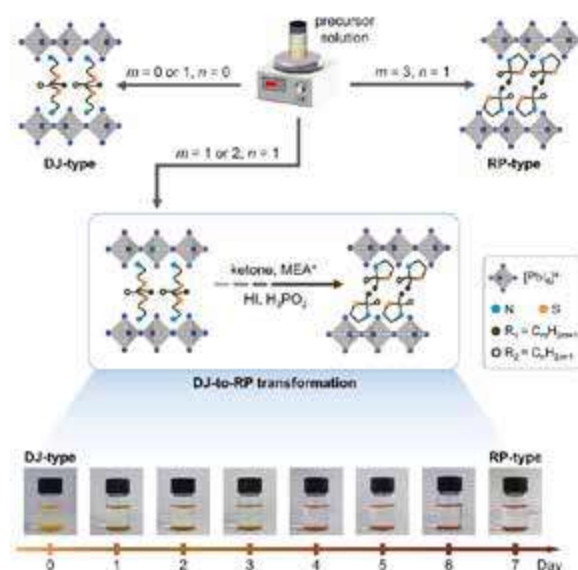
^bDepartment of Chemistry, York University, Toronto, ON M3J 1P3, Canada

*Corresponding author: yangzhy63@mail.sysu.edu.cn

Abstract

Two-dimensional metal halide perovskites (TMHPs) have emerged as prominent semiconducting materials in optoelectronic devices due to their compositional-dependent properties. While prior studies have primarily focused on the roles of cation type and chain lengths in TMHPs, we systematically investigate a new series of Dion-Jacobson (DJ) phase TMHPs incorporating dithioketal-containing organic cations.¹ Using X-ray crystallography and spectroscopic analyses, we reveal that the steric hindrance from longer branched groups distorts the structures and influences the photophysical behaviors of TMHPs. Further exploration of extended branched cations demonstrates a thermodynamically driven phase transition from DJ to Ruddlesden-Popper (RP) structures, accompanied with significantly different photophysical behaviors. These branched cations enable the fabrication of reduced-dimensional perovskite thin films with intense photoluminescence in the near-infrared region.² We further integrate these reduced-dimensional structures into near-infrared light-emitting diodes, where device performance strongly is strongly influenced by cation selection and inorganic layer dimensionality.

Keywords: metal halide perovskites, branched cation, crystal transformation, photophysics, light-emitting diodes



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UTILIZATION OF THE ELECTRON-RICH CARBORANES AS UNIQUE BASIC CATALYSTS IN ORGANIC SYNTHESIS

Peter Šrámel^a, Jan Vrána^a, Aleš Růžička^{a,*}

^aDepartment of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice, Czech Republic
Corresponding author: ales.ruzicka@upce.cz

Abstract

As a result of our recent research, a new class of polyhedral carboranes with unique basic properties was discovered. The heteroboranes are usually electronically deficient, however the coordination of suitable *N*-heterocyclic carbenes leads to an increase of the electron density in the cluster. Compounds with such a reversed polarity can subsequently act as relatively strong bases with a potential for synthetic application.¹

Based on our findings we decided to deeply examine the reactivity of these carboranes and utilize them as catalysts in organic synthesis. After our initially obtained positive results with base-induced enolization, we decided to examine a catalytic Michael addition. As a model reaction for the optimization, we choose a reaction of *trans*-chalcone with acetylacetone catalysed by borane **o-2**. Later we broadened the scope using various types of Michael donors and the acceptor with higher reactivity – β -nitrostyrene.

We proved **o-2** to be an effective catalyst for many substrates within the Michael addition, moreover, it was successfully used in various aldol condensations or even in the conditions of Robinson annulation. Currently we are working on the preparation of a modified version of **o-2** containing chiral carbene ligands, with a potential of application in the stereoselective synthesis.

Keywords: polyhedral carboranes, basic catalysis, Michael addition, Robinson annulation

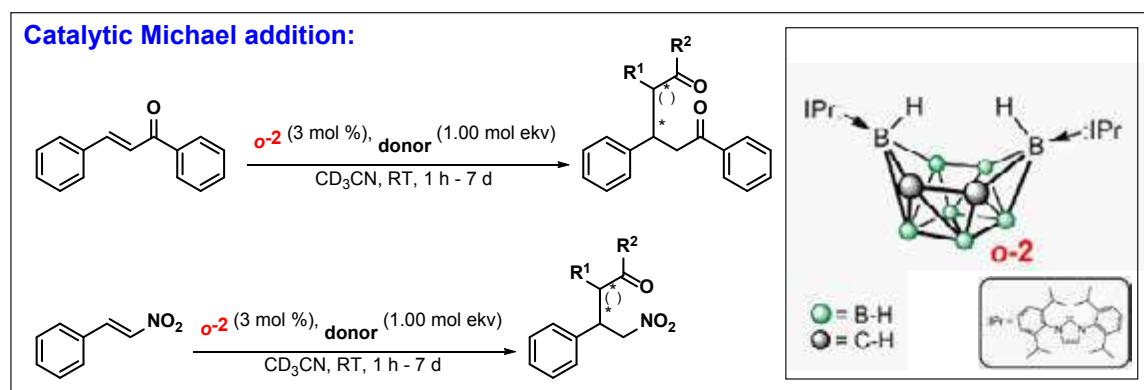


Figure 1. An overview of the developed conditions for the catalytic Michael addition and a structure of the tested catalyst – carborane **o-2**.

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DEVELOPMENT OF HYBRID COMPOUNDS OF METAL COMPLEXES AND ORGANIC COMPOUNDS WITH PEPTIDES THAT INDUCE PARAPTOTIC CELL DEATH IN CANCER CELLS VIA INTRACELLULAR CALCIUM SIGNALS

Shin Aoki^{a,b,c*}, Nozomi Narushima^a, Saki Sekiguchi^a, Toshifumi Tojo^{a,b}

^aFaculty of Pharmaceutical Sciences, Tokyo University of Science

^bResearch Institute for Science and Technology, Tokyo University of Science

^cResearch Institute for Biomedical Sciences, Tokyo University of Science

*Corresponding author: shinaoki@rs.tus.ac.jp

Abstract

Our research group has focused on the development of hybrid compounds of cyclometalated metal complexes and well-organized organic compounds with peptides, chromophore, and so on.¹⁾ Cyclometalated iridium(III) (Ir(III)) complexes such as *fac*-Ir(tolpy)₃ (tolpy = 2-(4'-tolyl)pyridine) are very stable in water and organic solvents and used as organic light emission diodes (OLEDs), cell imaging probes, and so on, due to their high stability and excellent emission properties such as large Stokes' shifts, high phosphorescent quantum yields, and long lifetimes (ms orders).¹⁾ We have reported on the design and synthesis of hybrid compounds of luminescent Ir(III) complexes with cationic peptide units (Ir(III) complex-peptide hybrids, IPHs) that function as the inducers of programmed cell death (PCD) in cancer cells and detectors of dead cells.¹⁻³⁾ In addition, triptycene derivatives functionalized with the similar cationic peptides (triptycene-peptide hybrids, TPHs) were synthesized and found to induce similar PCD in several cancer cell lines.^{4,5)} Importantly, the detailed mechanistic study of PCDs induced by IPHs and TPHs has disclosed that these hybrids induce the Ca²⁺ transfer from the endoplasmic reticulum (ER) to mitochondria, the membrane fusion between the ER and mitochondria, and vacuolization of intracellular organelles.^{2,4,5,6)} Therefore, PCD induced by IPHs and TPHs was referred to paraptosis II, because this PCD type is different from previously reported paraptosis I, which is induced by celastrol and negligibly involves membrane fusion between the ER and mitochondria. In this paper, these results will be reported.

Keywords: Cyclometalated iridium complexes; Triptycene, Peptide hybrids; Anticancer activity; Paraptosis

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INVESTIGATION OF THE CATION CAPTURING PROPERTY ON A Pd(II) COMPLEX WITH A BIS(1-(2-PYRIDYL)IMIDAZOLE-2-THIONE) LIGAND LINKED BY ALKYLDIETHER

Kenji Matsumoto*, Ryohei Tada, Yuya Fujita, Mao Hamada,
Takatoshi Kondo, Kei Sato

Department of Chemistry and Biotechnology, Faculty of Science and Technology, Kochi University.

*Corresponding author: matsuken@kochi-u.ac.jp

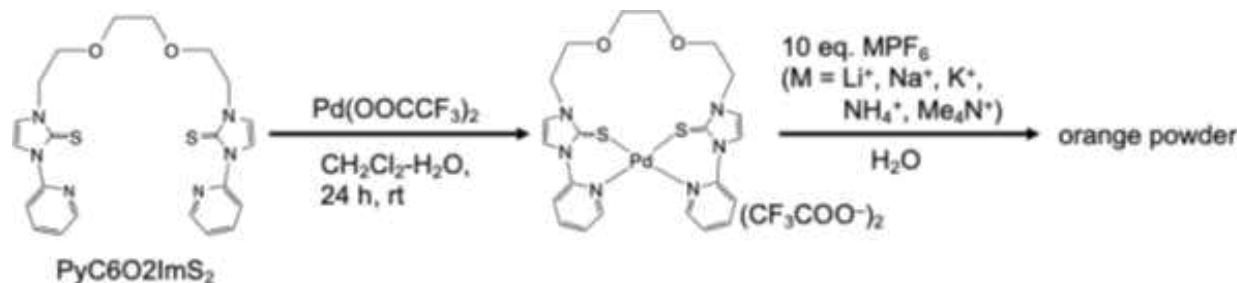
Abstract

Various ionophores such as crown ethers have been developed for ion sensing, ion extraction, organic synthesis and so on¹⁻³. Most of them are neutral or anionic because targeted metal ions have positive charges. Therefore, there is little report for cationic ionophores including heavy metal ions such as Rh(I) and Ir(I)^{4,5}. Recently, we have demonstrated that a palladium(II) complex with an alkyl-diether-bridged bis(1-(2-pyridyl)imidazole-2-thione) ligand (PyC6O2ImS₂, Scheme 1) is able to interact with ammonium ions in the solution state⁶. In this study, we have investigated the capturing property of the Pd(II)–PyC6O2ImS₂ complex for other cations such as alkaline and alkylammonium ions.

The palladium(II) complexes were synthesized by the reaction of the PyC6O2ImS₂ ligand with Pd(OOCCF₃)₂ and isolated by addition of excess MPF₆ (M = Li⁺, Na⁺, K⁺, NH₄⁺, Me₄N⁺) as an orange powder (Scheme 1). The ¹H NMR spectra of the palladium(II) complexes indicated the higher magnetic field shifts of the proton signals in the aromatic region compared to the Pd(II) complex without other cations. On the other hand, little shift of the proton signals in the alkyl region was observed. These results suggest that these cations interact with the aromatic rings of the Pd(II) complex.

Keywords: imidazolethione, ionophore, palladium complex, alkali ion, ammonium ion

Graphic / Image



Scheme 1. Synthesis of Pd(II)–PyC6O2ImS₂ complexes.

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UNEXPLORED FACETS OF LAYERED MATERIALS: NEW LOOKS TO OLD FACES

Luis R. De Jesús Báez^{a,*}, Jayanti Sharma^a, Alysson Bermudez^a,

^aUniversity at Buffalo

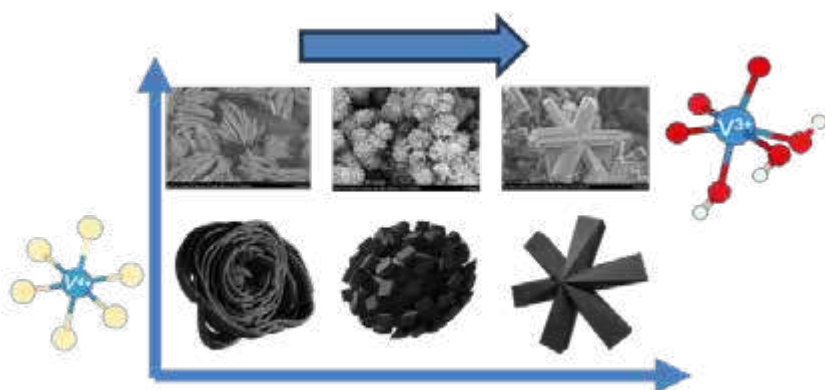
*Corresponding author: ldjesus@buffalo.edu

Abstract

The discovery and development of new materials tailored to a specific function remain as one of the grand challenges for materials' scientists. To this end, layered materials have been extensively studied due to the sundry of properties that emerge from chemical and physical modifications. Unfortunately, little is still known of the fundamental requirements to generate pronounced and tailored alterations to the electronic structure upon dimensional reduction or functionalization of their active sites. Comprehensive nanoscale characterization is essential to understand how the loss of 3D structural coherence and further modifications of the surface, induced because of ion intercalation, exfoliation to 2D sheets, or functionalization of the basal planes, alter the electronic structure of these materials which translates into physical properties. In this talk, I will discuss the use of layered VS_2 structures as seed to nucleate VOOH nanostars. We explore the relationship between the changes in morphology with fundamental changes in the electrochemical behaviour of the material. We observe a transformation from intercalation of Na ions to pseudocapacitive behaviour. Furthermore, we explore changes and describe synthetic conditions that allow the precise control of ligand modification on Fe-based layered double hydroxides as novel catalysts. With these modifications, we seek to understand changes in the capabilities of these materials to serve as pollution remediation catalysts, especially for emergent pollutants.

Keywords: inorganic synthesis, energy storage, sustainability, XAS

Graphic / Image



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METAL-ORGANIC FRAMEWORK ISOMERISM, SF₆ SORPTION AND FLUORESCENCE DETECTION OF ORGANOPHOSPHATES AND INSECTICIDES

Lars Öhrström^{a,*}, Hao Li^a, Francoise M. Amombo Noa^a, Michelle Åhlén^b, Zhejian Cao^c, Joakim Andréasson^a, Ocean Cheung^b,

^a Dept. of Chemistry and Chemical Engineering, ^b Dept. of Life Sciences, Chalmers University of Technology, SE-41296 Gothenburg, Sweden

^b Department of Materials Science and Engineering, Ångström Laboratory, Uppsala University, SE-751 03 Uppsala, Sweden

*Corresponding author: ohrstrom@chalmers.se

Abstract

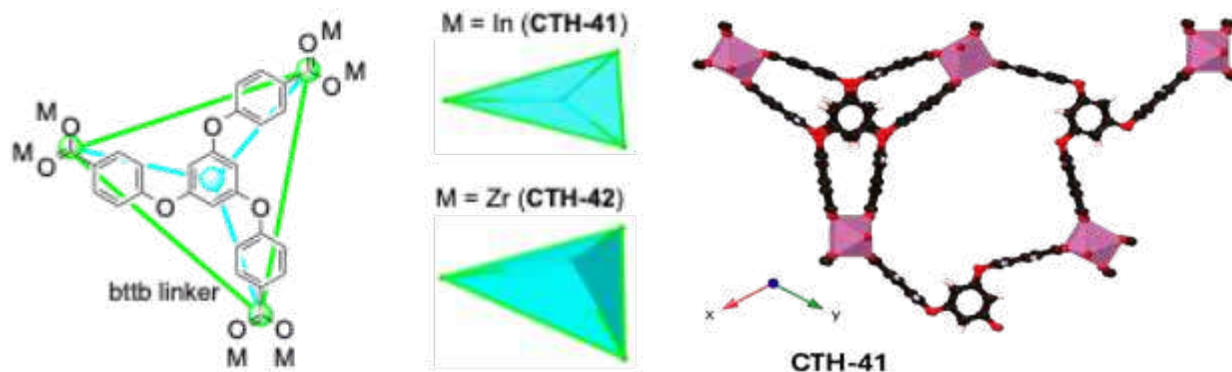
With In³⁺ the tritopic flexible linker 4,4',4''-(benzene-1,3,5-triyl-tris(oxy))tribenzoic acid (H₃bttb) gave a rod-Metal-Organic Framework with a topologically unique 3- and 4-connected net, [In₃(bttb)₂(OH)₃] CTH-41, that can be used to detect the chemical warfare mimic methyl paraoxon and the common insecticide permethrin by fluorescence quenching, but also highlighting the concept of framework isomers and the role of network topology analysis¹ in distinguishing them and determining their properties.

CTH-41 also showed affinity for SF₆ with a Langmuir area of 1587 m²/g while the new Zr⁴⁺ dot-MOF [Zr₆(bttb)₄(O)₄(OH)₄] CTH-42, with a Langmuir area of 527 m²/g, had affinity for CO₂ and forms the unusual 3-, 12-connected **llj**-net based on a different configuration of the flexible bttb linker.

The puzzling absence of 3- and 12-connected Zr-MOFs in the Cambridge Crystallographic Database, CSD, we explain by the network topology mismatch between a perfect cuboctahedron, the preferred Zr-Secondary Building Unit, SBU, and a perfect triangular SBU.

I will also talk briefly about the IUPAC Adsorption Information Format: A Universal Standard Archive File for Adsorption Data.²

Keywords: Metal-Organic Framework, Network Topology, Fluorescence, Framework Isomers, Gas Sorption



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- See <https://adsorptioninformationformat.com>

SYNTHESIS, REACTIVITY, AND ANTICANCER ACTIVITY OF NEW N-HETEROCYCLIC THIONES AND SELONES

Daniel Rabinovich^{a,*}

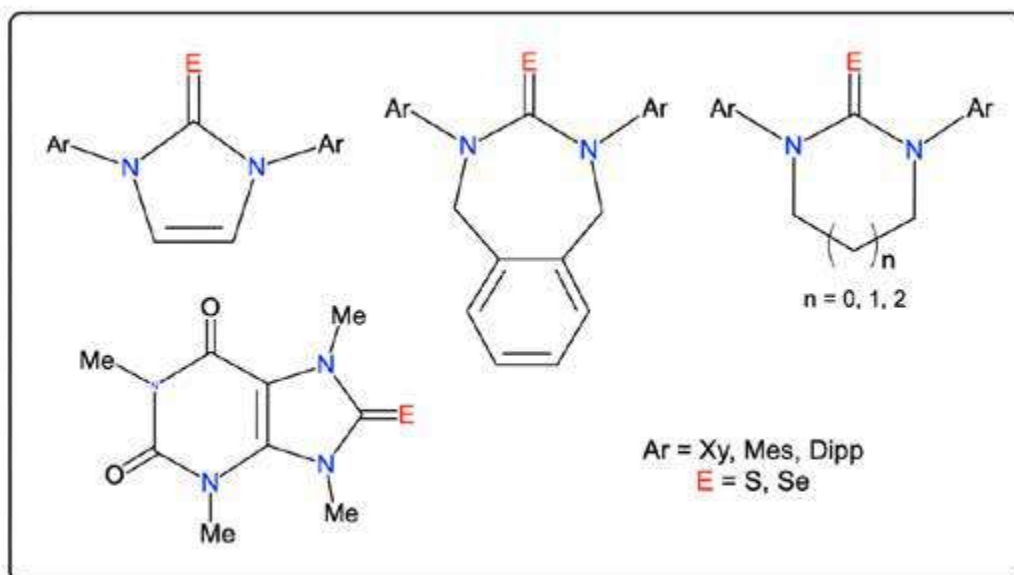
^aThe University of North Carolina at Greensboro

*Corresponding author: Dan.Rabinovich@uncg.edu

Abstract

N-heterocyclic thione and selone ligands have been extensively used in coordination chemistry, either directly as monodentate ligands or as versatile building blocks in a variety of chelating ligands, including soft analogues of the popular poly(pyrazolyl)borates or scorpionates.^{1,2} This presentation will outline recent advances in the synthesis and characterization of metal complexes supported by new sterically-demanding NHT and NHSe ligands. More specifically, an overview of the preparation of mercury(II), silver(I), palladium(II), and platinum(II) complexes will be presented, including the isolation of coordinatively unsaturated species and the isolation of compounds with unprecedented molecular structures in the context of NHT and NHSe coordination chemistry. Significantly, some of the silver compounds display potent anticancer activity, and will also be discussed in this presentation.

Keywords: N-heterocyclic chalcogenones, silver, mercury, palladium, anticancer drugs



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ADVANCING N-HETEROCYCLIC CARBENE COMPLEXES: SYNTHESIS, STRUCTURAL INSIGHTS, AND THEIR BIOLOGICAL APPLICATIONS IN ANTIMICROBIAL STUDIES

Yuen Lin Cheow^{a,*}, Kar Bee Choo^a, Jia Ming Khe^a

^aMonash University Malaysia

*Corresponding author: cheow.yuen.lin@monash.edu

Abstract

This presentation highlights recent advancements in the design, synthesis, and biological evaluation of N-heterocyclic carbene (NHC) complexes as promising agents for antimicrobial therapies. Two distinct studies focus on platinum, palladium, and silver NHC complexes with varying ligand architectures and substituents.

The first study explores platinum and palladium NHC complexes synthesized via a silver-mediated transmetalation approach, alongside unexpected nickel complexes prepared using a one-pot synthesis. Structural characterization, including single-crystal X-ray diffraction, revealed conformational properties, while biological assays demonstrated significant antimicrobial properties.^{1,2} A couple of platinum NHC complexes synthesized exhibited antimicrobial activities with MIC as low as 5 µg/mL, which are comparable to silver NHC complexes with renowned antimicrobial profiles.^{1,2} The second study focuses on bisimidazolium mononuclear and dinuclear silver(I)-NHC complexes with long alkyl chains. These complexes demonstrated promising antimicrobial activity with MICs as low as 0.12 µg/mL against Gram-positive and Gram-negative bacteria and fungi.³ The biscarbene structures exhibited reduced toxicity toward human keratinocyte cells, offering insights into optimizing bioactivity while minimizing side effects.

Together, these studies provide compelling evidence of the versatility and therapeutic potential of NHC complexes, underscoring their promise as next-generation antimicrobial agents.

Keywords: N-heterocyclic carbenes, Imidazolium salts, Metal carbene, Antimicrobial, Cytotoxicity

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SUPRAMOLECULAR TRIPLE-STRANDED HELICATES AS BUILDING BLOCKS FOR DISCRETE MOLECULAR CAGES

Thanh Nhan Nguyen^a, Hyojong Yoo^{a*}

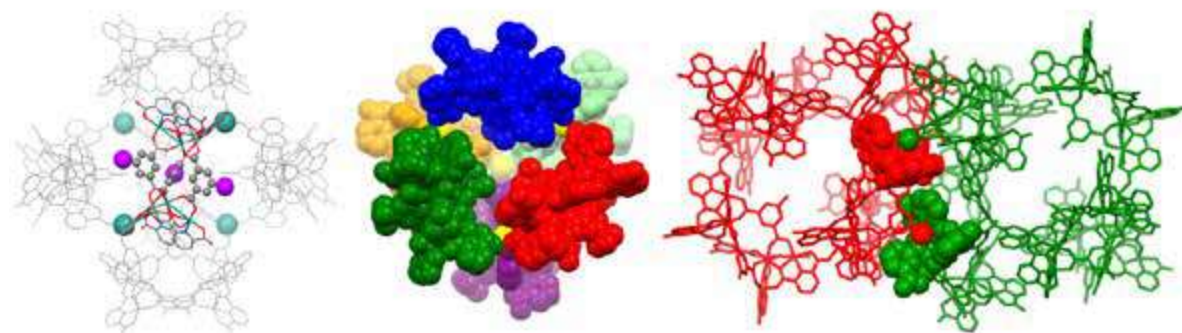
^a Department of Battery and Chemical Engineering, Hanyang University, Ansan, Gyeonggi-do 15588, Republic of Korea

*Corresponding author: hjhaha73@hanyang.ac.kr

Abstract

Creating hierarchical architectures with high functionality and complexity using supermolecular building blocks (SBBs) is getting interest compared with the conventional approach of using metal ions/clusters and organic ligands as building units. However, so far, the hierarchical architectures obtained from SBB approach are mainly one-dimensional (0D) and three-dimensional (3D) coordination polymers. Since our first success in the synthesis of supramolecular triple-stranded helicates (TSHs) assembled from two tetranuclear metal clusters (including four cobalt ions and three pyridine dicarboxylates) and three isophthalate bridging ligands, we found that when changing the substituent/functional group on C5 of the bridging ligands, various coordination platforms constructed from TSHs as SBBs have been obtained. Interestingly, when the substituents on C5 of isophthalate are methyl, *tert*-butyl, and bromo groups, TSHs can construct zero-order coordination cages (0D), which had not been reported before from SBB approach. In every single cage, six homochiral Co-TSH, either left (*M*)-handed or right (*P*)-handed, are connected by four linking cobalt atoms, forming M_6 or P_6 cages. Additionally, when changing metal ion from cobalt to nickel, nickel cages, which are isomorphous with cobalt cages, could be obtained. The crystal packing of racemic M_6 and P_6 cages in solid state indicates that methyl, *tert*-butyl, and bromo groups can act as guest units to be accommodated in the cone-shaped metal clusters (host) of an adjacent cage.¹⁻³

Keywords: Supramolecular building block (SBB), triple-stranded helicate, metallosupramolecular cage, host-guest interaction



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ISOINDOLINE-1,3-DIIMINE DERIVATIVES AND THEIR METAL COMPLEXES

Stanislava Majerova, Ales Ruzicka,

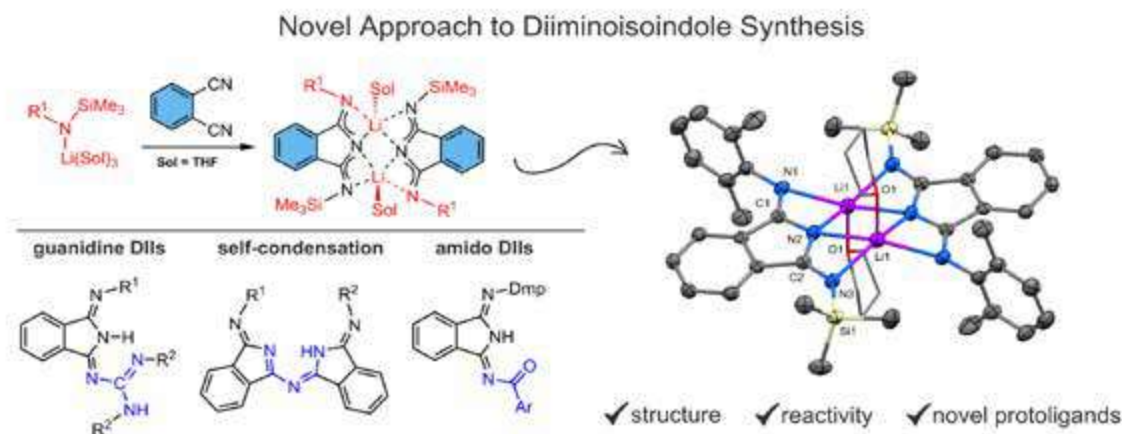
Department of General and Inorganic Chemistry, Faculty of Chemical Technology,
University of Pardubice, Studentska 573, 532 10 Pardubice, Czech Republic
* ales.ruzicka@upce.cz

Abstract

Phthalocyanines and its building blocks – isoindoline-1,3-diimines (diiminoisoindoles, DIIs), represent a structurally-diverse class of compounds with ability to make metal complexes and perform in various fields from medicine to photovoltaics and homogenous catalysis. According to the present study monosubstituted diiminoisoindoles,¹ their higher homologues, and complexes can be effectively prepared by an addition of silylated lithium amides to 1,2-dicyanobenzene followed by mild hydrolysis or a condensation. An addition of DII to carbodiimides or reactions of lithiated DIIs with acylchlorides give DII-guanidines and amido derivatives. Dynamic behavior and structure of all studied classes of compounds were investigated from the stereochemical point of view – possible E/Z-isomerization and dimerization (DIIs and amido derivatives), tautomerism (guanidines) and stability both in solution as well as in solid state. The resonance-assisted hydrogen bonds are present in all species, except reduced amides, predetermining them to be exceptional ligands in coordination chemistry.

Keywords: Diiminoisoindoline, Lithium, Prototropy, Complexes

Image



Acknowledgement: The work was supported by the Czech Science Foundation (No. 25-17434S) and Research infrastructure project CZ.02.01.01/00/23_021/0008593 (Innovative materials suitable for high added value applications (INMA)).

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REGULATING SHORT-RANGE CHEMICAL ORDERING AND LOCAL POLYHEDRAL CONFIGURATIONS IN Ni-Mo-P-B METALLIC GLASS

Zhongzheng Yao ^a, He Zhu ^{a*}, Jianrong Zeng ^{b,c*}, Si Lan ^{a*},

^a Herbert Gleiter Institute of Nanoscience, School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China.

^b Shanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Sciences, 201204 Shanghai, China.

^c Shanghai Institute of Applied Physics, Chinese Academy of Sciences, 201800 Shanghai, China.

*Corresponding author: hezhu@njjust.edu.cn; lansi@njjust.edu.cn.

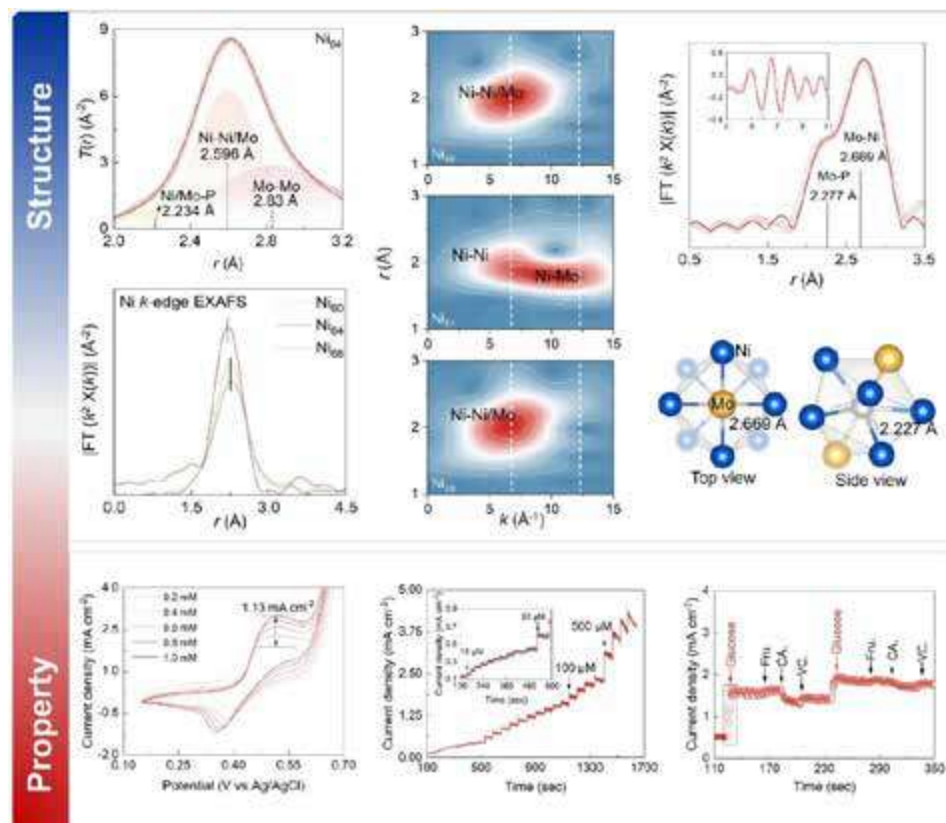
Abstract

The atomic structural characteristics of metallic glasses (MGs) can be described as short-range ordered polyhedral assembling into medium-range ordered cluster units in space. The diverse polyhedral types and flexible atomic connection modes endow their surfaces with abundant dangling bonds, thereby promoting electrochemical reaction processes. However, the lack of understanding about the complex structure of MGs hinders the tailoring of performance through structural regulation, which severely limits their further applications. Our study is to establish atomic-level structural regulate methods to optimize the electrochemical activity of MGs. Herein, we focus on the following aspects to elucidate the relationship between local structure and performance in MGs:

- (1) The significant efforts of minor compositional variations on the configurations of coordination polyhedras.
- (2) The influence patterns of local atomic arrangement on electrochemical activity.

As a result, our work establishes an atomic-scale structural engineering paradigm for MG design, advancing the understanding of structure-property correlations in amorphous materials.

Keywords: Metallic glass, regulate atomic structure, structure-property correlations



RUTHENIUM CATALYSTS FOR HYDROGEN PRODUCTION FROM FORMIC ACID: CATALYTIC EVALUATION AND MECHANISTIC INSIGHTS

Cassiem Joseph^{a,b*}, Rotondwa Mphephu^b, Andrew Swarts^b,

^aDepartment of Chemistry and Polymer Science, Stellenbosch University, Matieland, 7602

^bMolecular Sciences Institute: School of Chemistry, University of the Witwatersrand, South Africa

*Corresponding author: cjoseph@sun.ac.za

Abstract

The quest for sustainable energy solutions is steering the global research community towards innovations that can revolutionize the way we store and utilize energy. Among the many options, H₂ presents a highly promising path due to its potential for high energy yield and environmental friendliness.[1] However, the broad adoption of H₂ as an energy carrier is hindered by challenges associated with its storage and release. Compressed and cryogenic liquid H₂ storage methods pose economic and safety concerns. They require materials and infrastructure capable of withstanding extreme pressures and temperatures, which translates to high energy and material costs. Formic acid dehydrogenation processes are pivotal in the development of H₂ storage and release systems, offering a promising route for the on-demand production of H₂ gas, a clean energy carrier.[2-3] Formic acid, being a liquid at ambient conditions, serves as a convenient H₂ storage material due to its high hydrogen content and ability to release H₂ through dehydrogenation. The dehydrogenation of formic acid can be catalytically driven under mild conditions, which is advantageous for portable applications and where immediate hydrogen generation is required. Technological advancements in catalyst design and reaction engineering aim to optimize the efficiency, control, and safety of the dehydrogenation reactions, thereby enhancing the practicality of using formic acid in hydrogen storage systems. In light of this, we report on a series of pyridine-pyrazolyl Ru(II) complexes bearing different electronic and steric properties as catalysts for formic acid dehydrogenation (**Figure 1**). We demonstrated that the catalysts could dehydrogenate formic acid to CO₂ and H₂ in quantitative yields within 1 hour (5mmol FA, 5μmol catalyst loading, 3mmol HCOOK, 100°C) with TON's and TOF's of ~1030 mol_{FA dehydrogenated}/mol_{catalyst} and ~1230 h⁻¹ achieved respectively. Mechanistic studies for formic acid dehydrogenation are also reported.

Keywords: ruthenium catalysts, formic acid dehydrogenation, mechanistic studies

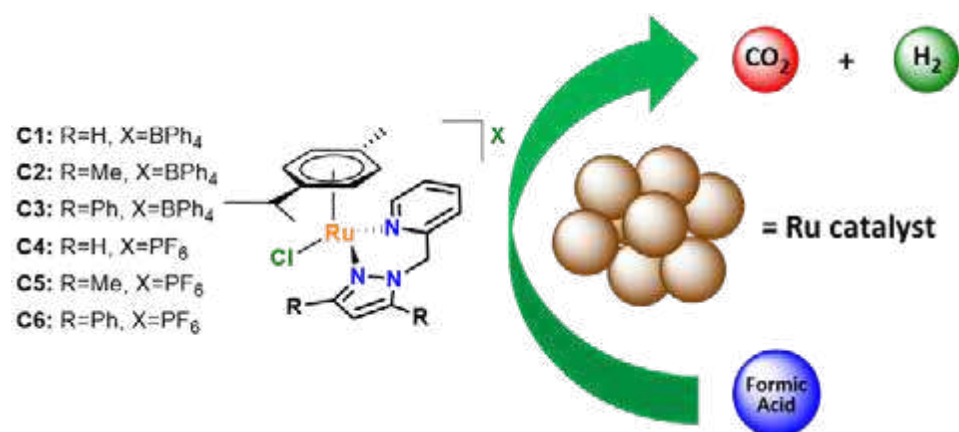


Figure 1: Formic acid dehydrogenation catalysed by Ru(II) pyridine-pyrazolyl complexes

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COPPER(II) SALPHEN COMPLEX AS A PROMISING OPTICAL SENSOR FOR 3-MONOCHLOROPROPANE-1,2-DIOL (3-MCPD) DETECTION

Nurul Huda Abd Karim ^{a,*}, Niza Norfitriah Mohd Zaini^a, Rabiatul Husna Mohd Nasir^a

^aDepartment of Chemical Sciences,

Faculty of Science & Technology

Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

*Corresponding author: nurulhuda@ukm.edu.my

Abstract

3-Monochloropropane-1,2-diol (3-MCPD) is a harmful contaminant formed during high-temperature processing of edible oils such as palm oil and olive oil, as well as in food products like soy sauce. Prolonged exposure to 3-MCPD has been linked to nephrotoxicity and reproductive toxicity, making its detection in food products a public health priority. While accurate, conventional analytical methods such as GC/MS and LC/MS are costly, labour-intensive, and unsuitable for on-site detection. Therefore, developing low-cost, rapid, and selective chemical sensors is critically needed. This study focuses on the synthesis, characterisation, and sensing performance of a copper(II) salphen complex as a novel optical sensor material for 3-MCPD. The complex was synthesised and characterised using spectroscopic techniques. A binding interaction study was carried out through UV-Vis titration, where the copper(II) salphen complex demonstrated a strong and consistent interaction with 3-MCPD, evidenced by a favourable binding constant (K_b). These results highlight the high potential of the copper(II) salphen complex as a selective and efficient sensor platform for 3-MCPD. A zinc(II) salphen complex was also synthesised and characterised for comparison. However, the zinc(II) complex showed weak and inconsistent binding with 3-MCPD, indicating inferior sensor performance relative to its copper(II) counterpart. In conclusion, this research underscores the promise of copper(II) salphen complexes as effective, accessible alternatives to traditional detection methods for monitoring 3-MCPD in food and oil products, paving the way for practical sensor development in the food safety industry.

Keywords: Metal salphen; 3-mcpd; optical sensor; metal complexes

DIOXYGEN ACTIVATION BY PALLADIUM(I) RADICALS

Samuel de Toro, Aliah El-Astal-Quirós, Cristina G. Yebra,* Ernesto de Jesús*

Departamento de Química Orgánica y Química Inorgánica, Instituto de Investigación Química “Andrés M. del Río”, Universidad de Alcalá, Campus Universitario, 28805 Alcalá de Henares (Madrid), Spain.

**Corresponding author: ernesto.dejesus@uah.es*

Abstract

Open-shell palladium complexes in oxidation states I and III provide alternative methods for single electron transfer (SET) bond formation.¹ Although monometallic palladium(I) metalloradicals are usually transient, the Chaplin and Ozerov groups independently isolated the stable palladium(I) two-coordinate complex $[\text{Pd}(\text{PrBu}_3)_2]^+$ in 2016.² Our group has achieved the kinetic stabilization of palladium(I) metalloradicals using bulky N-heterocyclic carbene (NHC) ligands. These $[\text{Pd}(\text{NHC})_2]^+$ complexes have been studied in the activation of small molecules by single electron reduction. Recent results from our group on the activation of dioxygen are reviewed in this communication.³ The reaction of $[\text{Pd}^{\text{I}}(\text{NHC})_2][\text{PF}_6]$ complexes (**1**) with dioxygen results in the formation of palladium(II) superoxides by transfer of the unpaired electron from the palladium center to the coordinated dioxygen molecule. In the absence of additional ligands, the uptake of dioxygen to form three-coordinate palladium(II) superoxido complexes $[\text{Pd}^{\text{II}}(\text{NHC})_2(\eta^1\text{-O}_2)][\text{PF}_6]$ (**2**) is reversible. However, the introduction of external ligands facilitates the stabilization of the dioxygen binding and the formation of stable four-coordinate palladium(II) superoxides $[\text{Pd}^{\text{II}}(\text{NHC})_2(\eta^1\text{-O}_2)(\text{L})][\text{PF}_6]$ (**3**). The reactivity of the superoxido radical can be modulated through the modification of the nature of the NHC and additional ligands. A discussion of the chemistry of these superoxides will be undertaken, with particular attention to EPR and paramagnetic NMR studies, thermodynamic data, and DFT calculations.

Keywords: Transition-metal radicals, dioxygen activation, N-heterocyclic carbene ligands, paramagnetic NMR spectroscopy.

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INNOVATIVE NANOSTRUCTURED DERIVATIVES OF ZINC(II) AND COPPER (II) PHTHALOCYANINE LIGATED WITH PIPERIDINE FOR PHOTODETECTION APPLICATIONS

Furkan Isik^{a,b}, Kevser Harmandar^c, Devrim Atilla^c, Betul Canimkurbey^{b,e,*}

^a*Institute of Accelerator Technologies, Ankara University, Ankara, Turkey*

^b*Department of Electrical and Electronics Engineering, Department of Physics, UNAM – Institute of Materials Science and Nanotechnology and The National Nanotechnology Research Center, Bilkent University, Ankara 06800, Turkey.*

^c*Gebze Technical University, Department of Chemistry, 41400, Gebze, Kocaeli, Turkey.*

^e*Department of Physics, Faculty of Polatli Science and Art, Ankara Hacı Bayram Veli University, Ankara 06900, Turkey.*

**Corresponding author: betul.canimkurbey@hbv.edu.tr*

Abstract

Organic photodetectors have garnered significant attention for their potential in low-cost, flexible optoelectronic applications. Phthalocyanines (Pcs), due to their unique electronic feature, exceptional flexibility to chemical modifications and stability, are promising candidates for such devices. However, their tendency to aggregate and limited solubility constrain film formation and device efficiency. This study aims to develop and evaluate novel Zn(II) and Cu(II) phthalocyanine derivatives functionalized with tetra piperidine groups to enhance solubility, suppress aggregation, and improve photodetection performance. The target Pc derivatives were synthesized via nucleophilic aromatic substitution and cyclotetramerization reactions. Their structures were studied by implementing Fourier-transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR) and matrix-assisted laser desorption/ionization time-of-flight mass spectroscopy (MALDI-TOF) while the optoelectronic properties were determined using ultraviolet-visible absorption spectroscopy (UV-Vis), fluorescence spectroscopy, electron-spin resonance spectroscopy (ESR) and cyclic voltammetry (CV). The performance of the metal-semiconductor-metal photodetectors implementing the synthesized Pc derivatives were examined by voltage-current measurements under optical excitation. The Zn(II) Pc-based photodetector device shows an order of magnitude higher photoconductivity of 1.56×10^{-4} mA/cm² compared to 3.17×10^{-5} mA/cm² of the Cu(II)Pc device, both at 10 V and 87.4 mW/cm². The devices made from Zn(II)Pc and Cu(II)Pc exhibited favorable photodetector performance, with responsivities of 2.3×10^{-5} mA/W for Zn(II)Pc and 1.3×10^{-5} mA/W for Cu(II)Pc. Additionally, these devices demonstrated high photo-to-dark current ratios, with values of 117 for the Zn(II)Pc device and 63 for the Cu(II)Pc device. Moreover, they showcased fast rise and decay time constants of 61 ms and 96 ms, respectively, for the Zn(II)Pc device, while the Cu(II)Pc device has rise and decay constants of 89 ms and 440 ms. The introduction of tetra piperidine ligands successfully enhanced the solubility and suppressed aggregation of MPc compounds, resulting in improved photodetector performance. Zn(II)Pc, in particular, demonstrated superior sensitivity and faster photoresponse, highlighting its potential for next-generation organic optoelectronic devices.

Keywords: Phthalocyanine, organic MSM photodetector, piperidine, photoresponse

IONIC FUNCTIONALIZED CO(II) SALICYLALDIMINATO COMPLEXES AS RECYCLABLE CATALYSTS FOR THE COUPLING OF CO₂ AND PROPYLENE OXIDE

Juanita L. van Wyk^{a*}, Ts'epo R. Tumeli^a

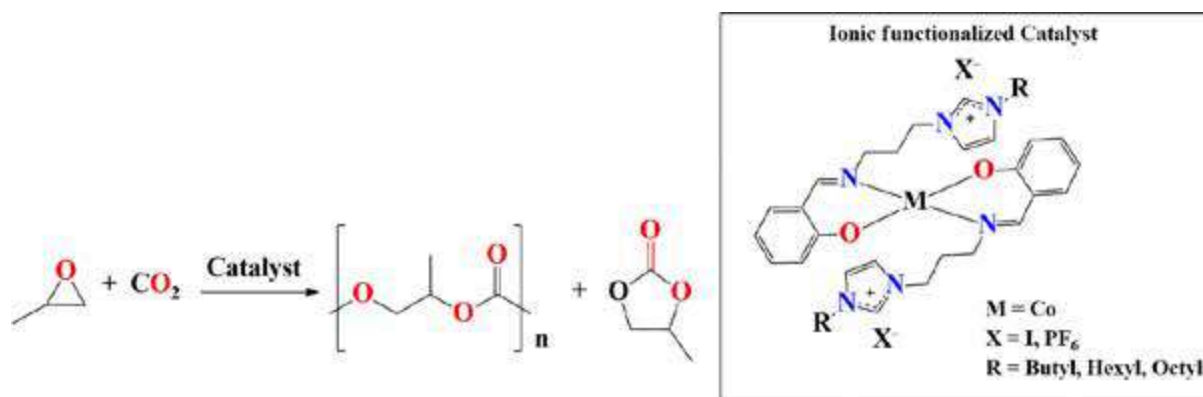
^a*School of Chemistry University of the Witwatersrand, Private Bag 3, Wits, 2050.*

**Corresponding author: Juanita.vanwyk@wits.ac.za*

Abstract

The coupling of CO₂ and epoxide is a catalytic process that has attracted increasing attention both industrially and in academia because it utilizes CO₂, which is abundant, bio-renewable and nontoxic C1 feedstock. This process yields polycarbonates which are biodegradable polymers that can potentially be applied as replacement for non-biodegradable plastic as well as cyclic products which have found application as solvents in lithium-ion batteries [1]. Transition metal catalysts have been shown to produce highly active homogenous catalytic systems in the presence of a suitable cocatalyst which is typically anionic in nature. In recent years multifunctional transition metal catalysts have been developed in which an ionic group incorporated on the ligand backbone functions as co-catalyst [2]. Multifunctional catalysts could potentially be utilized with ionic liquids to develop a biphasic catalytic process that would allow catalyst recycling which is usually a problem for homogeneous catalytic processes. This work is focused on the synthesis and characterization of ionic functionalized Co (II) complexes which are evaluated as catalysts in the coupling of CO₂ and propylene oxide in a biphasic catalytic process using ionic liquids as one of the solvents. The presentation will focus on experiments to develop a biphasic catalytic system as well as the catalytic performance of the Co (II) ionic functionalized complexes as for CO₂ and PO coupling.

Keywords: multifunctional catalysts, carbon dioxide transformation, biphasic catalysis, ionic liquids



Scheme 1: Coupling of CO₂ and propylene oxide using ionic functionalized Co(II) complexes.

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SYNTHESIS, AND BIOLOGICAL EVALUATION OF BENZIMIDAZOLE-BASED Cu(II) COMPLEXES: SPECTRAL, DFT, AND DOCKING INSIGHTS

Muhamad Azwan Hamali^a, Mohd Fadhilzil Fasihi Mohd Aluwi^{b,c},

Nur Amira Zulkifli^a, Maslinda Musa^d, Amalina Mohd Tajuddin^e, Karimah Kassim^{f*}

^a Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia

^b Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang Al-Sultan Abdullah, Lebuhraya Tun Razak, 26300, Gambang, Kuantan, Pahang Darul Makmur, Malaysia.

^c Centre for Bio-Aromatic Research, Universiti Malaysia Pahang Al-Sultan Abdullah, Lebuhraya Tun Razak, 26300, Gambang, Kuantan, Pahang Darul Makmur, Malaysia.

^d School of Biology, Faculty of Applied Sciences, Universiti Teknologi MARA, Shah Alam, 40450 Shah Alam, Selangor, Malaysia.

^e Atta-ur-Rahman Institute for Natural Product Discovery (AuRIns), UiTM Kampus Puncak Alam, 42300 Bandar, Puncak Alam, Selangor, Malaysia

^f Institute of Science, Universiti Teknologi MARA, 40450 Shah Alam, Malaysia

*Corresponding author: karimah@uitm.edu.my

Abstract

Lung cancer remains the leading cause of cancer-related deaths worldwide. The increasing incidence of cancer, coupled with the growing resistance of cancer cells to existing therapies, underscores the urgent need for the development of new and more effective anticancer agents^{1,2}. A series of Cu(II) complexes derived from benzimidazole-based ligands were synthesized and thoroughly characterized using spectral (FTIR, UV-Vis), analytical, and electrochemical techniques. The shifting of $\nu(\text{C}=\text{N})$ infrared band to lower wavenumber by 30-40 cm^{-1} , as well as the absence of $\nu(\text{-OH})$ indicate the chelation of copper ion with the ligand via imine N and phenolic O donor atoms^{3,4}. Furthermore, the electronic spectra of the Cu(II) complexes displayed broad absorption bands in the range of 649–652 nm, corresponding to d–d electronic transitions further support the complexation. Theoretical calculations were conducted using DFT at B3LYP/6-311G(d,p) level of theory revealed low energy band gap of the Cu(II) complexes (0.4680- 0.4871 eV) suggested that these complexes are reactive in nature⁵. Meanwhile, cytotoxicity studies against A549 lung carcinoma revealed that both Cu(II) complexes exhibited significantly higher antiproliferative activity (27-22 μM) compared to their corresponding ligands (62-56 μM). Furthermore, the molecular docking between the compounds and the MPP-9 protein (PDB ID: 5I12) showed low binding energies (-9.3 to -8.2 Kcal/mol) and with multiple stabilizing interactions correspond with the cytotoxicity result observed *in vitro*.

Keyword: Benzimidazole; Copper complex; DFT; Molecular docking; cytotoxicity; Schiff

SYNTHESIS, CHARACTERIZATION, AND ANTICANCER ACTIVITY OF COPPER(II) CHITOSAN FUNCTIONALIZED IMIDAZOLE-2-THIOSEMICARBAZONES

Hari Sharan Adhikari^{a,b,*}, Rameshwar Adhikari^{b,c,d}, Paras Nath Yadav^c

^a Pashchimanchal Campus, Institute of Engineering, Tribhuvan University, Pokhara, Nepal

^b Nepal Polymer Institute, Kathmandu, Nepal

^c Central Department of Chemistry, Tribhuvan University, Kathmandu, Nepal

^d Research Center for Applied Science and Technology, Tribhuvan University, Kathmandu, Nepal

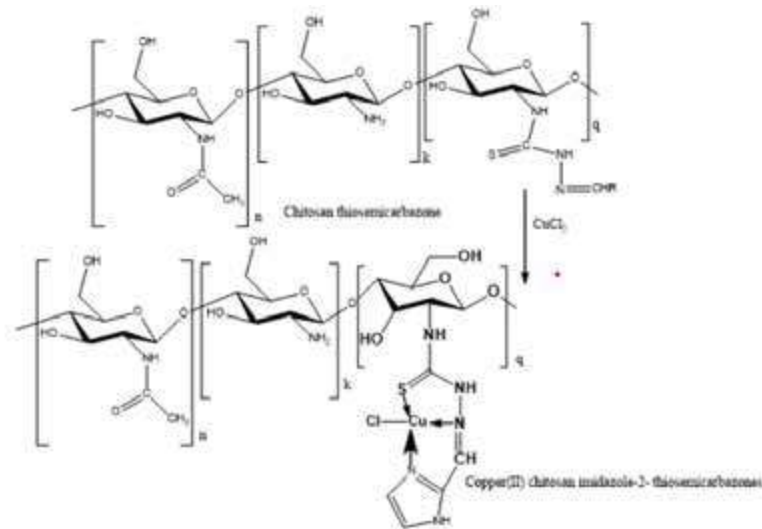
*Corresponding author: adhikaripkr687@gmail.com

Abstract

The coordination behavior of new batch synthesized chitosan imidazole-2-thiosemicarbazones tailored from both the low molecular weight commercial chitosan and high molecular weight crab shell chitosan was confirmed by Fourier Transform Infrared (FT-IR) and magnetic susceptibility measurements. Chlorine content in the complexes was estimated by potentiometric titration technique. The study showed the tridentate NNS tridentate coordination with copper (II) ion in a square planar orientation with the remaining valence satisfied by coordination with chloride ion. The MTT assay studies showed an enhancement in the anticancer activity of these chitosan thiosemicarbazone ligands upon their coordination with copper(II) ions against the human breast cancer (MCF-7) cell line in vitro. The minimal cytotoxicity of both the ligands and complexes against the normal mouse embryonic fibroblast (NIH3T3) cells revealed the selective attraction of these biomaterial chitosan derivatives towards the cancer cells with non-toxicity to healthy cells. There was only a marginal effect of molecular weight (M_w) and degree of deacetylation (DDA) of chitosan upon the anticancer activity of these chitosan derivatives. [1-2]

Keywords: Anticancer activity; Chitosan; Chitosan functionalized imidazole-2-thiosemicarbazones; Coordination behavior; Copper(II) chitosan functionalized imidazole-2-thiosemicarbazones

Graphical Image:



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QUANTIFYING THE ELECTRONIC PROPERTIES OF N-HETEROCYCLIC CARBENE LIGANDS USING SELENIUM NMR SPECTROSCOPY

Mohamad Shazwan Shah Jamil^{a,*}, Alan K. Brisdon^b

^aDepartment of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 Johor Bahru, Johor, Malaysia.

^bDepartment of Chemistry, The University of Manchester, M13 9PL, Manchester, United Kingdom.

^cAffiliation author W.

*Corresponding author: shazwan.shah@utm.my

Abstract

N-heterocyclic carbenes (NHCs) are common ancillary ligands in organometallic compounds that are used to alter the electronic and steric properties of a metal centre. To date, various NHCs have been synthesised with different electronic properties, which can be done by modifying the backbone or changing the nitrogen substituents group. The electronic properties (electron-donating and electron-accepting) of NHC ligands play a vital role in their bonding with transition metals, thereby influencing the selectivity and reactivity in catalytic processes¹. A number of methods have been developed that allow the electronic properties of NHCs to be quantified and compared. Some of these probes include infrared spectroscopy, nuclear magnetic resonance spectroscopy and electrochemical². Herein, we report a systematic modification of NHCs by the inclusion of fluorine substituents and examines the use of selenium-NHC compounds to measure the π -accepting ability of these fluorinated NHC ligands. Evaluation of the ^{77}Se NMR chemical shifts of the selenium adducts reveals that fluorinated NHCs have higher chemical shifts than the non-fluorinated counterparts, IMes and IPH. Higher ^{77}Se NMR chemical shifts values indicate a stronger π -accepting ability of the NHC ligands. The findings of this study suggest that the presence of fluorine atoms has increased the π -accepting ability of the corresponding NHC ligands. This work supports the advantage of the ^{77}Se NMR chemical shifts of selenium-NHC compounds for assessing the influence of fluorine substituents on NHC ligands³.

Keywords: N-heterocyclic carbene, ligand, electronic properties, NMR



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CROSS-COUPLING OF PYRIDINES VIA C–O ACTIVATION: DIVERGENCE AT THE CROSSROADS OF SINGLE- AND TWO-ELECTRON PATHWAYS

Ting-Hsuan Wang^{*a}, Chen-Hsun Hung^b, Jiun-Shian Shen^{b,c}, Tiow-Gan Ong^{*b,c}

^a Hubei Key Laboratory of Processing and Application of Catalytic Materials, Huanggang Normal University, Huanggang (China)

^b Institute of Chemistry, Academia Sinica, Taipei (Taiwan)

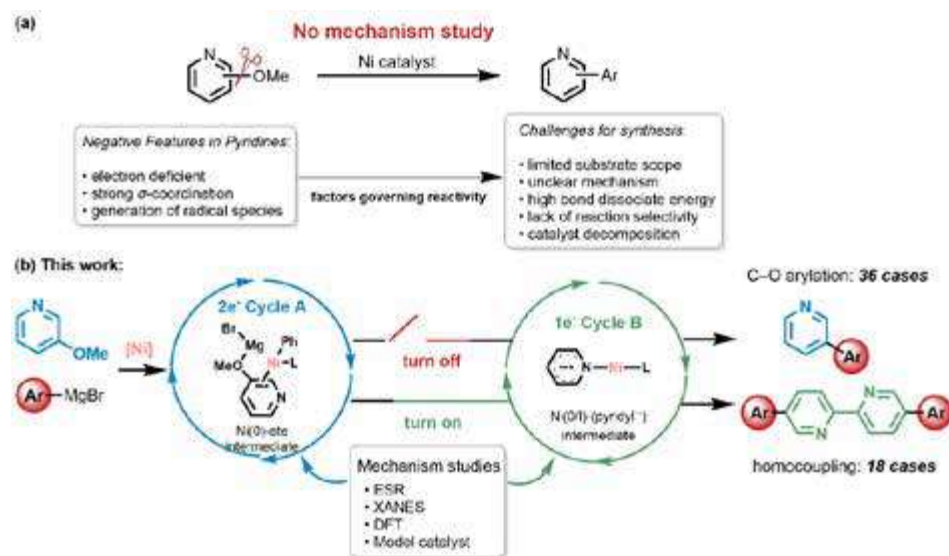
^c Dept. of Chemistry, National Taiwan University, Taipei (Taiwan)

*Corresponding author: tinawang7747@hgnu.edu.cn, tgong@gate.sinica.edu.tw

Abstract

The C–O bond activation in aryl ether derivatives offers a greener route by avoiding the need for halogenated electrophiles. Despite privileged scaffolds found in functional materials and pharmaceutical compounds, the inherent stability and electron deficiency of pyridine limit their utility in direct C–O functionalization and often lead to elusive side reactions. In this work, we report detailed mechanistic analysis concerning the nickel mediated C–O transformation of pyridyl methyl ethers. Supported by DFT calculation, X-ray absorption spectroscopy (XAS), electron spin resonance (ESR) and model catalyst, two distinct catalytic cycles were elucidated (i) the cycle A, responsible for C–O arylation via on a Ni(0)/Ni(II) redox manifold and (ii) the cycle B, involving key Ni(0/I)-pyridine radical cage species that promotes pyridine-pyridine homocoupling. These mechanistic insights were applied to substrate scope studies, allowing switchable catalysis for selective pyridine arylation and bipyridine synthesis.

Keywords: C–O arylation • metal–ligand redox cooperativity • nickel • pyridine • heterocycles



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NEW IRIIDIUM(III) COMPLEX BEARING WITH (E)-N-CYANO-N-(2,6-DIFLUOROBENZYL)-N'-(PYRIDIN-2-YL)FORMIMIDAMIDE ANCILLARY LIGAND

Nurul Husna As Saedah Bain^a, Noorshida Mohd Ali^{a,*}

^a Department of Chemistry, Faculty of Sciences and Mathematics, Universiti Pendidikan Sultan Idris, 35900 Tanjong Malim, Perak, Malaysia

*Corresponding author: noorshida@fsmt.upsi.edu.my

Abstract

The selection of ancillary ligands to be utilized in heteroleptic iridium(III) complexes significantly influences their chemical, spectroscopic, and luminescent properties hence playing a pivotal role in tailoring these complexes for specific applications. This study aims to synthesize a new heteroleptic iridium(III) complex bearing with new formimidamide base ancillary ligand for blue efficient phosphorescence. Formimidamide-based ancillary ligands were derived from the 1,2,4-triazolium salt during complexation with the iridium atom, resulting in the formation of complex $[\text{Ir}(\text{dFppy})_2(\text{L})]$ (where dFppy is cyclometalated 2,4-difluorophenylpyridine and L is (E)-N-Cyano-N-(2,6-difluorobenzyl)-N'-(pyridinyl)formimidamide ligand). Spectroscopic studies confirmed the formation of the new complex, as shown by a strong $\nu(\text{C}\equiv\text{N})$ stretching band at 2223 cm^{-1} in the IR spectrum, the disappearance of the singlet protons from the starting 1,2,4-triazolium salts in the ^1H NMR spectrum, and the appearance of a nitrile carbon signal at 117.9 ppm in the ^{13}C NMR spectrum. X-ray single crystallographic study confirmed the iridium was coordinated to two cyclometalated phenylpyridine ligands and a pyridinylformimidamide ancillary ligand in a distorted octahedral geometry. The UV-Vis absorption spectrum exhibited a broad, low-energy peak at $\lambda_{\text{abs}} = 375\text{ nm}$ ($\epsilon = 5900\text{ M}^{-1}\text{ cm}^{-1}$) in the visible region, attributed to $^1\text{MLCT}$ and $^3\text{MLCT}$ transitions, from which the energy gap between the HOMO and LUMO was estimated. The simulated structural and spectroscopic of the new complex was assessed with a basis set of B3LYP/6-31G(d,p), and LanL2DZ at the ground state. The HOMO–LUMO band gap energy of 3.88 eV is relatively large, highlighting the potential of this complex for use in phosphorescent devices like organic light-emitting diodes (OLEDs).

Keywords: Iridium(III) complex; Formimidamide ligand; Ancillary ligand; DFT; HOMO–LUMO

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CHIRALITY TRANSFER IN COORDINATION-DRIVEN SUPRAMOLECULAR CAGES

Jacopo Tassarolo^{a,*}

^a Dept. of Chemistry, Chonnam National University, Republic of Korea

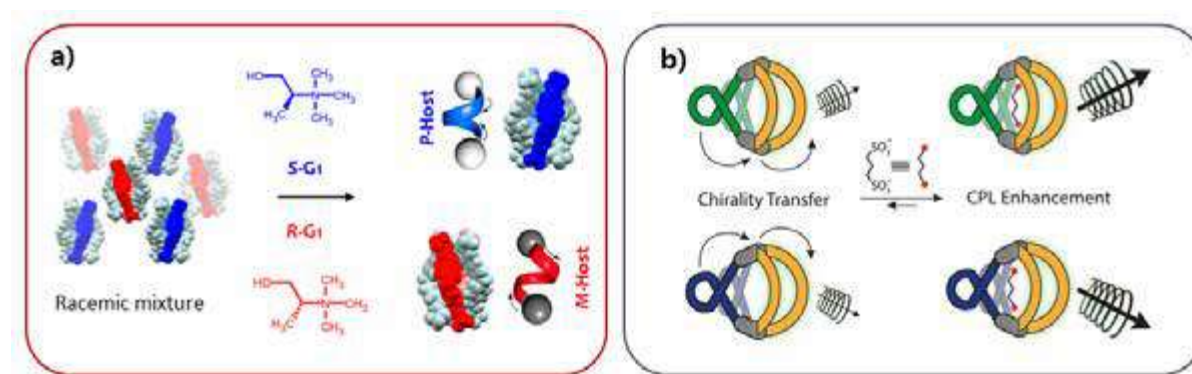
*Corresponding author: jacopo@jnu.ac.kr

Abstract

Metal-mediated self-assembly of supramolecular architectures has been proven to be an efficient tool for developing new materials with well-defined shapes and geometries. Ligand design and choice of metal allow to obtain a large variety of compounds with nanosized pockets able to host specific guest molecules [1]. At the same time, functions deriving from the metal center, such as lanthanide emission [2], or from the organic ligand, for instance chromophores or photoswitches [3], can be implemented. Herein we combine chirality and emission properties from different building blocks, to achieve circular polarized luminescence (CPL) in supramolecular assemblies via guest-to-host [2] (Figure 1a) or ligand-to-ligand chirality transfer [4] (Figure 1b). The latter is based on the combination of multiple ligands following non-statistical processes to yield heteroleptic assemblies displaying CPL. The presence of a cavity allows to study molecular recognition, while combining multiple ligands allows or to tune the properties of the systems by exchanging the building blocks in a modular fashion.

Keywords: Self-assembly, Chirality, Supramolecular Cages, Metal-organic

Graphic / Image



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ZINC(II)-BASED COORDINATION POLYMERS FOR CHEMICAL SENSORS AND CATALYSTS

Haeri Lee*

Department of Chemistry, Hannam University, Daejeon, 34054, South Korea

**Corresponding author:: haeri.lee@hnu.ac.kr*

Abstract

Catalysts play a crucial role in enhancing the efficiency of chemical reactions in a field of environmental, industrial, and biological applications. In particular, heterogeneous catalysts provide the advantage of easy separation from the reaction solution. Polymeric metal compounds, which have less solubility in organic solvents, are applied as heterogeneous catalysts to initiate organic reactions. With the increasing focus on environmental concerns, sustainable and alternative energy sources like biodiesel derived from fats and soybean oils have gained prominence over fossil fuels. Biodiesel production involves a transesterification process, which requires specific catalysts, sensitive to moisture and pressure conditions. In our research, we synthesized discrete Zn(II)-based complexes and used them as catalysts in the transesterification reaction. The ligand and metal complexes were analyzed by spectroscopic techniques and characterized their crystal structures by X-ray diffraction method. Subsequently, the catalytic activities of these complexes in the transesterification reaction were examined.

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ZWITTERIONIC STIBINIDENE IN REDOX CATALYSIS

Yi Chen Chan, Oriol Planas

Department of Chemistry, Imperial College London, London, United Kingdom

*Corresponding author: y.chan@imperial.ac.uk

Abstract

The upmost position of transition metals (TMs) in catalytic processes stems from their relative ease to coordinate substrates and manoeuvre between oxidation states. Yet, the supply of noble metals (NMs; e.g. Pd, Rh, Ir, Pt) is in danger due to increasing geopolitical clashes, remarkably increasing their cost. This, together with their environmental footprint urge chemists to focus on infusing their key properties to more abundant main group elements (MGs), like the pnictogen family (Pn, group 15).^{1,2} Herein, we showcase the isolation of low valent cationic antimony (Sb) species in +1, +2 and +3 oxidation states stabilised by an anionic *bis*(*N*-heterocyclic Carbene)borate ligand to give an overall charge-neutral complexes. Computational studies indicate the cationic character of the stibinidene center and its unique electronic properties, which resemble the tetrylones of group 14. Stoichiometric oxidative addition and reductive elimination reactivity of the zwitterionic stibinidene complex led to the exploration of redox catalytic hydrodefluorination reactions, marking a significant milestone for cationic pnictinidenes catalysing a redox transformation and providing reactivity beyond the conventional *N,C,N*-pincer ligand used in low-valent pnictogen redox catalysis

Keywords: Pnictogen, Cationic Stibinidene, Redox Catalysis, Hydrodefluorination

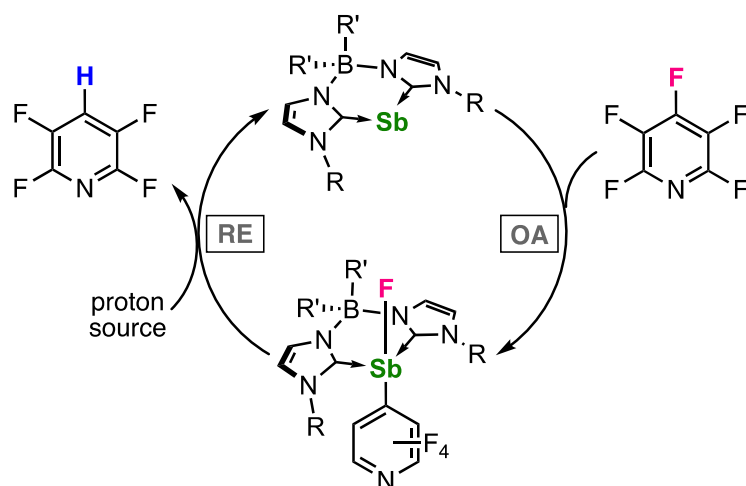


Figure 1. Zwitterionic Stibinidene-Catalyzed Hydrodefluorination of Polyfluoroaromatics through a Sb(I)/Sb(III) catalytic cycle.

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SYNTHESIS AND RAMAN SPECTROSCOPY OF CONFINED CARBYNE AND GRAPHENE NANORIBBONS

Yingzhi Chen^a, Weili Cui^a, Huiju Cao^a, Kunpeng Tang^a, Yanghao Feng^a, Lei Shi^{a,*}

^aSun Yat-sen University, Guangzhou, China.

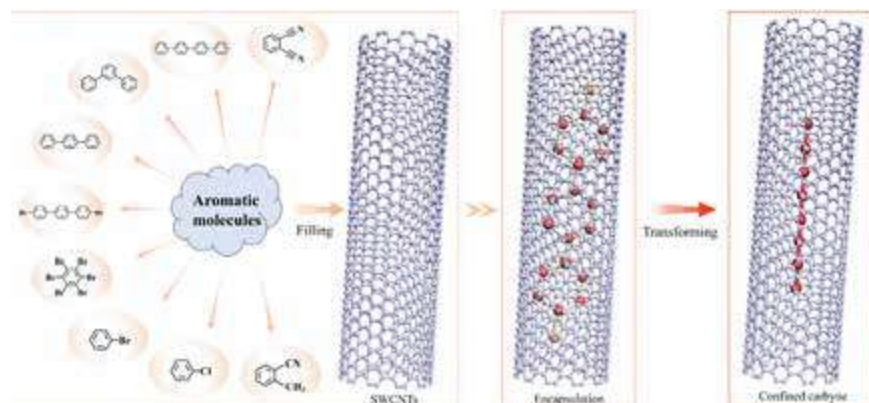
*Corresponding author: shilei26@mail.sysu.edu.cn

Abstract

One-dimensional carbon nanomaterials, including quasi-one-dimensional carbon nanotubes, graphene nanoribbons, and fully one-dimensional carbon chains, have become hot topics in the field of nanotechnology. One-dimensional carbon chains have unique electron orbitals that give them superior performance, with theoretical predictions suggesting that their mechanical, electrical, and thermal properties even surpass those of graphene. However, the highly unstable structure of carbon chains limits independent existence at ambient conditions, posing significant challenges for experimental research. On the other hand, graphene nanoribbons overcome the limitations of graphene's zero band gap by controlling the edge structure and width, which makes them a potential material for semiconductor applications. The 1D nanospace of carbon nanotube is an ideal nanoreactor for synthesis of nonexistent or unusual materials, e.g., previously we have synthesized ultra-long linear carbon chains (carbyne) [1-4]. Thanks to the confinement of the carbon nanotube and Raman Spectroscopy, the evolution (or reaction) of precursor molecules under high temperature or high pressure can be studied in detail now. Here, our recent results discovered that some precursor molecules with/without hexatomic rings can be converted into graphene nanoribbons [5-7], whereas some aromatic molecules can be transformed into linear carbon chains, as shown in the attached Figure [8]. These unusual phenomena are beyond the conventional chemical reaction. In addition, many kinds of 1D elemental or compound chains can be obtained by using the same confined synthesis, which paves the way to create a library of novel 1D materials that do not exist or are yet to be explored.

Keywords: Carbyne, Graphene nanoribbons, Carbon nanotubes, Raman spectroscopy

Graphic / Image



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TWO-DIMENSIONAL HEXAAMINOPHENYL CONDUCTIVE METAL-ORGANIC FRAMEWORK FOR HIGH-PERFORMANCE LITHIUM-SULFUR BATTERIES

Yongsheng Fu*,

Key Laboratory for Soft Chemistry and Functional Materials, Ministry of Education, Nanjing University of Science and Technology, Nanjing 210094, China

*Corresponding author: fuyongsheng@njust.edu.cn

Abstract

Lithium-sulfur batteries (LSBs) are the most promising next-generation energy storage batteries due to their high theoretical energy density (2600 Wh kg^{-1}), high theoretical cathode capacity of 1675 mAh/g , natural abundance of sulfur and environment friendly. However, during the discharge process, the shuttle effect caused by the generated lithium polysulfides (LiPSs) and slow sulfur reduction reaction (SRR) kinetics lead to low sulfur utilization, resulting in insufficient sulfur reduction and reduce specific capacity and rate performance. Herein, a highly crystalline hexaaminophenyl conductive metal-organic framework (Ni-HAB) is in situ grown on the surface of carbon nanotubes (CNT) using a defect-induced adsorption and two-dimensional confinement approach. Then Ni-HAB@CNT hybrid material is employed as a modifying layer on the PP separator to suppress polysulfide shuttle and catalyze its conversion. The highly crystalline Ni-HAB two-dimensional conductive MOF possesses ordered micropores with a diameter of approximately $8 \text{ \AA}$, enabling the entrapment of polysulfides while permitting the transport of lithium ions. In addition, the Ni(II) planar tetrahedral coordination structure in Ni-HAB minimizes spatial hindrance between catalytic sites and polysulfides. The significant overlap of $\text{dz}^2(\text{M})-\pi(\text{ligand})$ orbitals enhances electron delocalization. Combined with the inherent long-range electrical conductivity of CNTs, this imparts exceptional adsorption, catalytic, and conductive properties to the Ni-HAB@CNT hybrid material. As a result, the combined blocking and facilitating effects of Ni-HAB@CNT significantly enhance the battery's electrochemical performance.

Keywords: lithium-sulfur battery, shuttle effect, catalysis

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SYNERGISTIC SOLVENT EXTRACTION OF LANTHANOIDS WITH TRADITIONAL LIGANDS (4-ACYLPYRAZOLONE AND BIDENTATE NITROGEN BASES) IN A NONTRADITIONAL DILUENT CONFIRMED BY NMR

Maria Atanassova Petrova

*University of Chemical Technologies and Metallurgy,
Department of General and Inorganic Chemistry,
8 Kliment Okhridski blvd., 1756 Sofia, Bulgaria
Corresponding author: ma@uctm.edu

Abstract

The phenomenon observed in the field of solvent extraction chemistry, whereby the combined use of two extractants results in the extraction of a metal ion species with a significantly enhanced efficiency compared to the additive effect observed when they are used separately, is referred to as a synergism.^{1,2} The synergistic solvent extraction of La(III), Eu(III) and Lu(III) with a chelating extractant 4-benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one (HL/HP) and neutral bidentate heterocyclic amines, such as 1,10-phenanthroline (S1 (phen)) or 2,2'-bipyridine (S2 (bipy)) in an ionic liquid of the imidazolium family $[C_1C_4im^+][Tf_2N^-]$ was investigated. Synergistic effects have been observed to result from the formation of a ternary complex in the organic phase, particularly in cases where the ligand S is a neutral synergistic agent. Examples include $La(L)_2(S2)_2$, $Eu(L)_3(S2)$, $Lu(L)_x(S2)_2$, as well as $La(L)_3(S1)_2$, $Eu(L)_2(S1)$ and $Lu(L)_3(S1)_x$. The parameters of the solvent extraction process were determined and the influence of the synergistic agent on the extraction process was discussed.³ Additionally, the synergistic increase and separation factors were determined. The equilibrated organic phases were analysed using ^1H NMR spectroscopy to elucidate the synergism in an extraction mechanism. In addition, very weak interaction between the two extracting molecules (HL+1,10-phen or HL+2,2'-bipy) presented in the organic phase was also detected. However, this observation should not cause any influence on the synergistic process.⁴ The role of the ionic diluent in complexation processes and selectivity was investigated with the employment of the two synergistic agents for various metal s-, p-, d- and f-cations in the Periodic table, with almost 22 metal ions.

Funding: This study is funded by the Bulgarian Science Fund through the Grant Agreement № KP-06-H69/5(2022), “Green twist to synergistic solvent extraction and separation of rare earth metals”.

Keywords: lanthanoids, synergistic extraction, 4-benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one, 1,10-phenanthroline, 2,2'-bipyridine, NMR, separation factors.

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SYNTHESIS AND CHARACTERISATION OF DIPYRROLIC LIGANDS AND THEIR METAL COMPLEXES

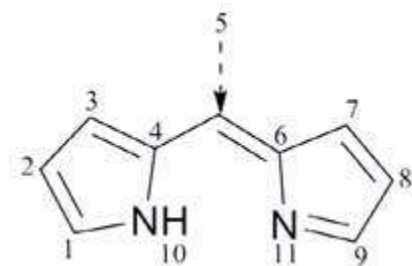
Sadhna Mathura^{a*}

^aMolecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa

*Corresponding author: sadhna.mathura@wits.ac.za

Abstract

Dipyrromethenes (dipyrins) are versatile class of organic ligands having an array of applications. Inherently simple in structure, the dipyrin motif comprises two pyrrole rings fused by a methine bridge. The simplicity of this structural motif allows for an array of possible functionalization to optimize its strong fluorescence and photostability properties. These optimized properties serve many applications, especially when dipyrins are complexed to transition metal ions. Applications include use in bioimaging, optoelectronic technologies, sensors and photodynamic treatments. There is therefore growing interest in examining metal complexes containing functionalized dipyrromethene cores. Examining how the functionalized moieties and the transition metal ions influence the fluorescence and photostability properties may improve application design and usefulness of these complexes. This work therefore reports on the synthesis and characterization of selected dipyrins functionalized at the *meso*-position¹, their complexation to selected metal ions and the possible influence of both on their optoelectronic properties.



1. Dipyrromethene (dipyrin) motif

Keywords: dipyrromethenes, dipyrins, transition metals, functionalization

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CATALYTIC OXIDATION OVER IRON INCORPORATED MESOPOROUS MOLECULAR SIEVES (Fe-JLU-15)

K. Chellal¹, K. Bachari², F. Sadi¹

¹Laboratory for the Physico-chemical Study of Materials and Application to the Environment. Faculty of Chemistry.
U.S.T.H.B. Algeria

²Scientific and Technical Research Center in Physico-Chemical Analysis, Algiers, Algeria

*Corresponding author: khachellal@gmail.com

Abstract

Fe-containing mesoporous materials (Fe-JLU-15) prepared by using semifluorinated surfactant as a template, has been synthesized by microwave-hydrothermal (M-H) process. The characterization by several techniques of this material has shown that several iron species could be identified at the surface of the pore walls of the mesoporous silica and the surface area and pore volume of the Fe-JLU-15 are lower than those prepared by conventional-hydrothermal synthesis. The catalytic activity of this materials was tested for the phenol hydroxylation and wet phenol oxidation with H_2O_2 under mild reaction conditions ($P = 1\text{ atm}$ and $T = 40^\circ\text{C}$). The effect of pH, $\text{H}_2\text{O}_2/\text{PhOH}$ molar ratio and stability of the catalyst on the oxidation process was also investigated. Phenol oxidation and H_2O_2 decomposition show that Fe-JLU-15 is active and stable in aqueous solution. The total amount of dissolved iron is less than 5 wt% of the iron initially contained in the catalyst. In phenol hydroxylation, catechol and hydroquinone were observed as the major products, with a high selectivity for catechol ($\text{CAT}/\text{HQ} = 2.7$ and 63.5 % phenol conversion).

Keywords: Fe-JLU-15 Phenol Iron Oxidation Hydroxylation

GENERAL SYNTHESIS OF OXIDES/OXIDES INTERFACED SPHERES FOR SOLAR H₂ FUEL

Muhammad Waqas*

Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

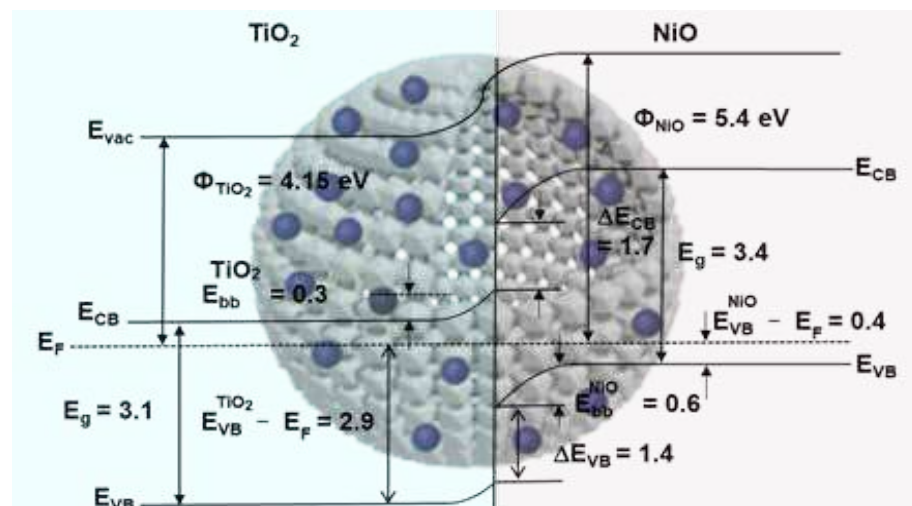
**Corresponding author: muhammad.waqas@kfupm.edu.sa*

Abstract

Oxide-on-oxide interfaces present significant interest for technological applications due to their unique chemical bonding, which facilitates superconductivity, magneto-electric coupling, and the quantum Hall effect.¹⁻² Conventional oxide-on-oxide systems exhibit a non-ideal distribution of isomorphic epitaxial structures, resulting in decreased interface stability and catalytic effectiveness. This study introduces a comprehensive synthesis method for continuous interfaces between oxides, specifically NiO and various metal oxides such as TiO₂, Fe₂O₃, and Co₃O₄. The approach yields ultra-dispersed NiO and exhibits significant interfacial polymorphism within concentrated spheres of metal oxides. NiO/MO spheres are synthesized through self-assembly utilizing cationic dodecyltrimethylammonium bromide, resulting in a thick carbon layer abundant in C=O and OH⁻, followed by rapid calcination in air. X-ray diffraction and electron microscopy are essential techniques for elucidating material formation mechanisms. This study demonstrates that NiO/TiO₂ p-n heterojunction spheres exhibit superior performance compared to conventional catalysts in solar hydrogen evolution. The approach is anticipated to facilitate the rational synthesis and analysis of contiguous interfacial chemical bonding organizations within and outside complex spheres.

Keywords: Structural Engineering, Interfacial Chemistry, inorganic oxides, band-energy alignment, heterogenous catalysis

Graphic: Band alignment at the heterojunction interface of n-type (TiO₂) and p-type (NiO) semiconductors



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CHIRAL-METAL ORGANIC FRAMEWORKS (CMOF) BASED CIRCULARLY POLARIZED FLEXIBLE SPIN LIGHT EMITTING DIODES

Mujahid Mustaqeem^{*a}, Mohammed Ashraf Gondal^{a,b}

^aInterdisciplinary Research Center for Hydrogen Technologies & Carbon Management, KFUPM, Dhahran 31261, Saudi Arabia.

^bDepartment of Physics, King Fahd University of Petroleum and Minerals (KFUPM), Dhahran 31261, Saudi Arabia.

^{*}Corresponding author: mustaqeem.mujahid@gmail.com

Abstract

Flexible spintronics is a crucial emerging field in next-generation wearable and innovative electronic technology. Traditionally, spintronics relies on external magnetic fields and ferromagnetic contacts to achieve spin-polarized carriers. This makes it challenging to realize flexible spin devices due to the inherently bulky and rigid constituent materials. To overcome these drawbacks, we propose a strategy for fabricating flexible spin light-emitting diodes by integrating self-assembled monolayer (SAM) of P3HT-COOH, chiral metal-organic framework (MOF), quantum dots (QDs), and polyethylene terephthalate substrate. The chiral Europium-based metal-organic framework utilized as a spin-injection layer through a chiral-induced spin selectivity (CISS) mechanism can effectively polarize the emitting light. The SAM (P3HT-COOH) layer significantly enhances the device stability and light intensity compared to conventional PEDOT: PSS layer-based devices, while the QDs layer serves as the bright emitter. Our device achieves an estimated external quantum efficiency (EQE) with a polarization degree (P_{CP-EL}) of $\pm 21.86\%$. Furthermore, the degree of polarization changes with stable emission under various bending radii. This approach enables circularly polarized luminescence (CPL) and tuneable polarization degrees to be simultaneously free from external magnetic fields or ferromagnetic contacts. The obtained result offers a promising alternative in the field of flexible spintronics and builds up an additional means to manipulate the physical properties of spin devices. This study is significant and timely for potential applications in flexible electronics and quantum information processing, which are expected to attract academic and industrial interests.

Keywords: Chiral-MOF, Flexible-Spin LEDs, Circular Polarized Light (CPL), Degree of Polarization, Chiral Induced Spin Selective (CISS).

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ORGANONICKEL COMPLEXES BASED ON THE ALKYL-CHAIN EFFECT FOR HIGHLY EFFICIENT SOLAR-DRIVEN EVAPORATION AND ELECTRICITY

Jen-Shyang Ni^{a,b*}, Joanna S. Lin^a

^a Department of Chemical and Materials Engineering, National Kaohsiung University of Science and Technology (NKUST), Kaohsiung 80778, Taiwan

^b Photo-sensitive Material Advanced Research and Technology Center (Photo-SMART), NKUST, Taiwan

*Corresponding author: jsni@nkust.edu.tw

Abstract

Solar-steam generation (SSG) is a friendly environmental water treatment technology that resolves global water scarcity.^[1,2] The emergence of photothermal materials with broad absorption and photothermal conversion efficiencies (PTCEs) offers an effective approach to enhancing SSG performance. In this study, the organonickel complexes tying different alkyl-chain lengths were developed for constructing the solar interfacial evaporator. These complexes with unique intervalence charge transfer-induced second near-infrared (NIR-II) absorption exhibit broad absorption from visible to NIR-II regions and increase sunlight utilization. After adsorbed on filter paper to form evaporators, their photothermal conversion temperatures can rise over 180 °C under 1064 nm of laser irradiation (1 W cm⁻²), attributing to the complex's J-aggregation quenches radiative transition rate. The solar energy-to-vapor rates of the 3 mg-NiTh16 forming evaporator achieve 1.72 and 1.69 kg m⁻² h⁻¹ for deionized water and seawater, respectively, under one solar irradiation (1 kW m⁻²). Herein, over 100% efficiencies result from that network fiber holes of filter paper provide the capability to capture the incident sunlight and then reduce reflection losses and enthalpy, thereby enhancing the conversion of solar energy into heat.^[1] Under the irradiation of three suns, the NiTh16-based thermocouple can also present 440 mV of voltage, which has certain advantages in comparison with the reported system. This investigation will not only offer the design strategy for enhancing SSG performance through alky-chain modification but also expand the organometallic materials for solar energy-powered desalination and electricity applications.

Keywords: SSG, photothermal, desalination, near-infrared, J-aggregation.

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EXPLORING HISTATINS: THE RELATIONSHIP BETWEEN THE COORDINATION CHEMISTRY AND ANTIMICROBIAL ACTIVITY

Emilia Dzień^{a,*}, Joanna Wątył^a, Daniela Valensin^b, Miquel Adrover^c, Agnieszka Matera-Witkiewicz^d,
Magdalena Rowińska-Żyrek^a

^a Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland.

^b Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Via A. Moro 2,
53100 Siena, Italy.

^c Institut Universitari d'Investigació en Ciències de la Salut (IUNICS), Institut de Recerca en Ciències de la Salut (IdISBa), Departament de Química, Universitat de les Illes Balears, Ctra. Valldemossa km 7.5, E-07122 Palma de Mallorca, Spain.

^d Screening of Biological Activity Assays and Collection of Biological Material Laboratory, Wrocław Medical University Biobank, Faculty of Pharmacy, Wrocław Medical University, Borowska 211A,
50-556 Wrocław, Poland.

*emilia.dzien@uwr.edu.pl

Abstract

Antimicrobial peptides (AMPs) play a significant role in the innate immune system of living organisms. These small, positively charged peptides, typically containing up to 100 amino acids, are essential in defending against microorganisms by either killing them or preventing their growth. AMPs are gaining attention as potential therapeutic agents, often exhibiting stronger antimicrobial effects or enhanced action when interacting with metal ions. This interaction can disrupt microbial survival and virulence by depleting them of critical metal ions, a phenomenon known as “nutrition resistance.” Moreover, metal ions can improve the effectiveness of AMPs by altering their charge or structure.¹ Histatins, a type of small salivary peptide, belong to the cationic AMP group and are active against bacteria and fungi, particularly *Candida albicans*.²

We consider the relationship between the coordination chemistry and antimicrobial properties of Cu(II) and Zn(II) histatin complexes, using a range of analytical methods such as potentiometry, UV-Vis, CD, NMR, SAXS spectroscopy and antimicrobial activity assay. Cu(II) generally coordinates in a binding mode similar to albumin (except for histatin 4, which lacks the ATCUN motif), while Zn(II) can bind to the (i) carboxylate side chain of glutamic acid and two histidine imidazole groups or (ii) two histidyl residues, with the presence of polymorphic binding sites. The antimicrobial effectiveness of histatins and their complexes is significantly influenced by pH, and in most cases, Zn(II) coordination enhances their antimicrobial activity. Additionally, when histatins 3-4 and 5-8 bind to Zn(II) ions, they undergo structural changes, becoming more α -helical.^{3,4}

Acknowledgements

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Keywords: antimicrobial peptides, histatins, Zn(II) and Cu(II) complexes, thermodynamics stability

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TRIMETALLIC PALLADIUM-BASED CATALYST SUPPORTED ON SCHIFF BASE CONJUGATED GRAPHITIC CARBON NITRIDE IN HYDROGEN GAS GENERATION

Ai Ling Koh^{a*}, Ming Yueh Tan^a, Siew San Tan^a, Abdulkareem G. AlSultan^b, Nurul Asikin-Mijan^c, Yun Hin Taufiq-Yap^b,

^a*Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Kuala Lumpur.*

^b*Catalysis Science and Technology Research Centre (PutraCat), Faculty of Science, University Putra Malaysia, Serdang, 43400, Selangor, Malaysia.*

^c*Department of Chemical Sciences, Faculty of Science and Technology, University Kebangsaan Malaysia, Bangi, 43600, Selangor, Malaysia;*

*Corresponding author: kohal-wp20@student.tarc.edu.my

Abstract

Environmental pollution and the depletion of primary energy sources have increased the need for renewable energy. Formic acid dehydrogenation (FAD) facilitated by catalysts is one of the practical approaches for hydrogen gas production due to formic acid's high hydrogen storage capacity. In this project, different ratios of trimetallic palladium-based catalysts supported on Schiff base conjugated graphitic carbon nitride (SB-g-C₃N₄) managed to synthesize through the wet chemical reduction method. Among them, Pd_{0.5}Au_{0.2}Co_{0.3} catalyst was the most effective in hydrogen gas generation in FAD. The catalyst was characterized with Fourier Transform Infrared Spectroscopy (FT-IR), X-ray Powder Diffraction (XRD), Thermogravimetric Analysis (TGA), Field Emission Scanning Electron Microscopy (FESEM) and Brunauer-Emmett-Teller (BET) analysis. The XRD pattern of the catalyst showed a peak around 38°, matching the diffraction peaks of Au (111) (JCPDS: 01-089-3097), confirming the successful metallic formation via the wet chemical reduction method. Additionally, the Pd_{0.5}Au_{0.2}Co_{0.3} catalyst exhibited a decomposition temperature of approximately 766.8 °C, indicating high thermal stability. Besides, Pd_{0.5}Au_{0.2}Co_{0.3} also demonstrated excellent performance in formic acid dehydrogenation with relatively high turnover frequency (TOF) at ambient temperature. The high catalytic activity is proposed due to the strong electronegative group on the Schiff base in assisting the dissociation of the O-H of formic acid to form the hydrogen gas. In conclusion, catalysts supported by SB-g-C₃N₄ show potential for catalytic activity in FAD study and support global efforts in transitioning to cleaner energy sources.

Keywords: Carbon nitride, Formic acid dehydrogenation, Hydrogen gas, Trimetallic catalysts, Schiff base

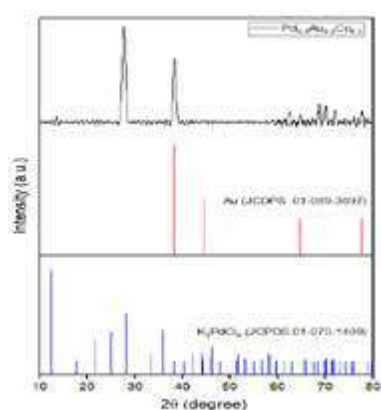


Figure 1. XRD patterns of Pd_{0.5}Au_{0.2}Co_{0.3} catalyst

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PHOTOSENSITISING AGENTS FOR ANTIBACTERIAL AND ANTICANCER TREATMENT: RUTHENIUM POLYPYRIDYL/SCHIFF BASE COMPLEXES

Kuan Teng Tan^a, Ke Hui Lee^b, Pei Yi Tan^a, Wei Meng Lim^c, Yun Khoo Liew^d, Chun Wai Mai^e, Lai Chun Wong^f, May Lee Low^a

^aFaculty of Pharmaceutical Sciences, UCSI University, Kuala Lumpur, Malaysia.

^bSchool of Postgraduate Studies, IMU University, Kuala Lumpur, Malaysia.

^cSchool of Pharmacy, Monash University, Selangor, Malaysia.

^dDepartment of Life Sciences, School of Pharmacy, IMU University, Kuala Lumpur, Malaysia.

^eCentre for Cancer and Stem Cell Research, Institute for Research, Development, and Innovation, IMU University, Kuala Lumpur, Malaysia.

^fDepartment of Pharmaceutical Chemistry, School of Pharmacy, IMU University, Kuala Lumpur, Malaysia.

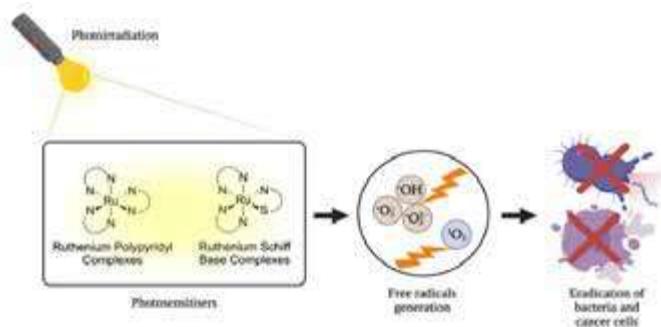
*Corresponding author: lowml@ucsiuniversity.edu.my

Abstract

Cancer remains a global threat attributed to its uncontrollable cell growth and metastasis, yet treatment options remain ineffective or trigger side effects against healthy cells.¹ Similarly, the emergence of multidrug-resistant bacteria urges the discovery of potent antibiotics to prevent possible complications such as sepsis.¹ Henceforth, alternative strategies for instance photodynamic therapy (PDT) has been researched extensively to enhance treatment efficacy, improve patient compliance and minimise side effects.¹ PDT involves the targeted delivery of photosensitiser to trigger oxidative stress, vasculature damage and activate immune system to eradicate cancer cells or bacteria.^{1,2} Ruthenium (Ru) complexes possess immense photoactivity which upon photoirradiation at specific wavelengths generates abundant reactive oxygen species.² Coordination of Ru with polypyridyl ligands or Schiff bases induces bathochromic shift of maximum absorption wavelength ($\lambda_{\max}$), enhances photostability, luminescence and Stokes shift, thus increasing overall cytotoxic effects.^{2,3} This project aims to develop bioactive Ru(II) metal complexes with synergistic effects for both cancer and bacterial infections, utilising advanced techniques for evaluation and potential combination therapy with cisplatin. Among tested compounds, $[\text{Ru}(\text{bpy})_2(\text{SB4CB})]\text{PF}_6$ and $[\text{Ru}(\text{bpy})_2(\text{SBFH})]\text{PF}_6$ displayed significant antibacterial effects against *Staphylococcus aureus*, which upon photoirradiation MIC values were both 16 μM ; and MIC values for non-photoirradiated samples were 16 μM and 8 μM respectively. For anticancer evaluation, $[\text{Ru}(\text{bpy})_2(\text{SB4CB})]\text{PF}_6$ demonstrated excellent cytotoxicity effects against MDA-MB-231 breast cancer cells and MeL28 melanoma cells, with IC_{50} values of 6.72 μM and 9.39 μM respectively in light conditions.

Keywords: Ruthenium polypyridyl complexes, Schiff bases, photodynamic therapy, antibacterial, anticancer

Graphic / Image



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IMPLICATIONS OF SYMMETRY AND ORIENTATION OF NAPHTHYL SUBSTITUENTS OF METALLOSALEN AND SALPN-BASED NAPHTHALENE COMPLEXES IN THEIR CO₂ ELECTROREDUCTION CAPABILITIES

Dalice M. Piñero Cruz^{a,b,*}, Christopher A. Samaniego-Rodriguez^{a,b}, Darién O. Kercado-Colón^{a,b}, Jemily Acosta-Mercado^{a,b}, Javier O. Rivera-Reyes^{a,b}, Alanys V. Luna-Ramírez^{a,b}, Yomaira Pagán-Torres^c, Miguel Sepúlveda-Pagán^c, John-Paul Jones^d

^a Department of Chemistry, College of Natural Sciences, University of Puerto Rico-Rio Piedras Campus, San Juan, PR 00925-253, USA

^b Molecular Science Research Center, University of Puerto Rico, 1390 Ponce de León, San Juan, PR 00926, USA

^c Department of Chemistry Engineering, University of Puerto Rico-Mayagüez Campus, Mayagüez, PR 00681-9000, USA

^d Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA

University of Puerto Rico-Mayagüez Campus, Mayagüez, PR 00681-9000, USA

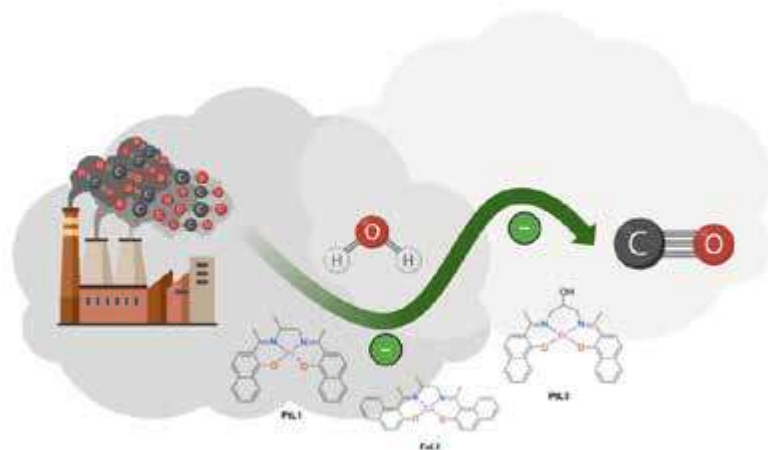
*Corresponding author: dalice.pinero@upr.edu

Abstract

Efforts to electrocatalytically reduce greenhouse gases such as carbon dioxide (CO₂) to convert it into value-added products is the ongoing subject of the research presented herein. In our research, the salen sites have been designed to anchor the desired metal ions in a semi-rigid square planar basal plane with the possibility of having axial coordination of ligands such as CO₂, which are thus the catalytic sites. We have identified that the nature of the metal center and the extension of the aromaticity on the ligand platform by use of the naphthyl group increases the metallosalen and metallosalpn-based complexes catalytic activity thus inducing the formation of several products. In this presentation results will be discussed on the synthesis, structural and catalytic activity of horizontal versus vertically aligned aromatic groups of metallosalen and salpn-based naphthalene complexes from Pd²⁺, Pt²⁺ and Cu²⁺. We report improvements in the CO Faradaic efficiency of >40% from most systems in the presence of water as a sacrificial proton source at a potential range of -2.5 V to vs. Fc/Fc⁺.

Keywords: electrocatalysis; CO₂ utilization; Schiff-base; DFT calculations, metallosalen complexes

Graphic / Image



RING OPENING POLYMERIZATION OF RAC-LACTIDE BY TRANSITION METAL COMPLEXES LIGATED BY AMINOMETHYLQUINOLINE DERIVED LIGANDS

Hyosun Lee

Department of Chemistry
Kyungpook National University
80 Daehakro, Bukgu, Daegu, 41566, Republic of Korea
*Corresponding author: hyosunlee@knu.ac.kr

Abstract

Green polymers such as biodegradable polylactide (PLA) and polycaprolacton (PCL), have been played a role of substitutes for petroleum-based materials. They are widely used in commodity, biomedical, pharmaceutical applications, and packaging industries. Specifically, transition metal complexes have been utilized as catalysts for the ring opening polymerization (ROP) of lactide (LA). Thus, we have synthesized transition metal complexes such as cobalt(II), copper(II), zinc(II) complexes supported by *N,N'*-bidentate aminomethylquinoline derived ligands, 2-(piperidin-1-ylmethyl)quinoline (L_{pmq}), 4-(quinolin-2-ylmethyl) morpholine (L_{qmp}). The characterization of the complexes was conducted using ^1H NMR, ^{13}C NMR, elemental analysis (EA), FT-IR and X-ray single crystal diffraction. Catalytic studies conducted with these complexes in the presence of the initiating reagent, lithium isopropoxide (LiO^tPr), showed their reactivity towards ring-opening polymerization (ROP) of *rac*-lactide (*rac*-LA) at 0 °C and 25 °C. In particular, the catalytic system [L_{qmp}] $CoCl_2$ /LiO^tPr resulted in over 95% conversion within 30 seconds using [*rac*-LA]:[(L_{qmp}) $CoCl_2$]:[LiO^tPr] ratio of 100:1:2 at 0 °C. Additionally, all complexes demonstrated hetero-enriched polylactides (PLAs) exhibiting superior heterotactic PLA ($P_r = 0.74$) at 0 °C, and the resulting PLAs displayed low molecular weights and a narrow range of polydispersity indices (PDI = 1.22–1.25).

Keywords: ring opening polymerization, *rac*-lactide, transition metal complex, heterotacticity, polydispersity indices

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DUAL TARGETING OF A549 LUNG CANCER SPHEROIDS USING RUTHENIUM(II) POLYPYRIDYL COMPLEX AND PARP INHIBITION

Haslina Ahmad^{a,b*}, Nur Ainie Yusoh^b, Martin R. Gill^c, Chia Suet Lin^b

^a Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

^b UPM-MAKNA Cancer Research Laboratory, Institute of Bioscience, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

^c Department of Chemistry, Faculty of Science and Engineering, Swansea University, Swansea, UK.

*Corresponding author: haslina_ahmad@upm.edu.my

Abstract

The use of 3D spheroid models for drug evaluation provides valuable insights into cytotoxicity and drug penetration¹, offering a more physiologically relevant representation of the tumor microenvironment compared to conventional 2D cultures. These models mimic the complexity and heterogeneity of clinical tumors, making them an effective platform for anticancer drug testing. Ruthenium(II) polypyridyl complexes (RPCs) have gained attention as potential anticancer agents due to their strong DNA-binding properties². Meanwhile, poly(ADP-ribose) polymerase (PARP) inhibitors have emerged as promising therapeutic molecules³. In our previous study, we demonstrated the synergistic effect of the RPC [Ru(dppz)₂(PIP)]²⁺ (dppz = dipyrdo[3,2-a:2',3'-c]phenazine, PIP = 2-(phenyl)-imidazo[4,5-f][1,10]phenanthroline), known as "Ru-PIP," in combination with the PARP inhibitor Olaparib in 2D monolayer cultures⁴. Here, we extend our investigation to a 3D lung cancer spheroid model to further assess the synergistic potential of Ru-PIP and Olaparib. A549 lung cancer spheroids were generated using the hanging drop technique, followed by spheroid growth inhibition assays and live/dead staining to evaluate treatment effects. A549 spheroids exhibited continuous growth over 15 days, validating their use as a 3D tumor model. Treatment with the Ru-PIP/Olaparib combination led to significant structural disintegration of the spheroids after 12 days, whereas spheroids treated with single agents remained intact, despite Ru-PIP alone inhibiting spheroid growth. Calcein AM/PI staining further confirmed that the combination induced greater cell death compared to single treatments. These findings highlight the potential of the Ru-PIP/Olaparib combination in overcoming resistance in 3D lung cancer spheroid models.

Keywords: Lung Cancer, Combination Therapy, Ruthenium, PARP inhibitor

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SUZUKI COUPLING OF TWISTED AMIDES: AN EFFECTIVE PD PRECATALYST STRATEGY

Yu-Hsiang Liu^a, Xhuan-Hao Kang^a, Yu-Chang Chang^{a*}

^aDepartment of Applied Chemistry, Providence University, Taichung 43301, Taiwan

Corresponding author: vickchang@pu.edu.tw

Abstract

We have developed a highly effective heteroleptic Pd(II) precatalyst, IPr-PdCl₂-P(tolyl)₂(OH), which is effective in catalyzing Suzuki couplings of unactivated aryl chlorides, benzyl chloride, and benzoyl chlorides.¹ Lately, we discovered that IPr-PdCl₂-P(tolyl)₂(OH) can be readily synthesized by reacting the PEPSI precatalyst IPr-PdCl₂-Pyridine with di(p-tolyl)phosphine oxide, consistent with the hard and soft acids and bases (HSAB) theory. Using IPr-PdCl₂-P(tolyl)₂(OH) as a precatalyst, we selectively cleaved the N-C(=O) bond, which exhibits partial double-bond character, in sterically demanding cyclic amines acting as electrophilic reagents. This facilitated the smooth participation of amides in the Suzuki cross-coupling reaction. Research on palladium-catalyzed oxidative addition of N-C(=O) bonds is limited in the literature² and has primarily focused on NHC-Pd-type precatalysts.^{3,4} Compared to the excellent NHC-Pd catalysts,³ our recently developed and highly effective precatalyst could reduce reaction time and lower the reaction temperature. The IPr-PdCl₂-P(tolyl)₂(OH)-catalyzed Suzuki couplings successfully transformed amides into aryl ketones using arylboronic acids as coupling partners. This study demonstrates that the IPr-PdCl₂-P(tolyl)₂(OH) is excellent at facilitating the oxidative addition step in cross-coupling reactions.

Keywords: Palladium precatalyst, Secondary Phosphine Oxide, N-heterocyclic carbene, Acylative Suzuki coupling, Amide



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SYNTHESIS, CHARACTERIZATION AND ANTITUMORAL ACTIVITY IN OVARIAN CANCER CELLS OF NEW GOLD(I) COMPLEXES.

^aAdam A. A. Sulaiman, ^bNaïke Casagrande, ^bCinzia Borghese, ^{a,c}Anvarhusein A. Isab,
^bDonatella Aldinucci

^aDepartment of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

^bMolecular Oncology Unit, Centro di Riferimento Oncologico di Aviano (CRO), IRCCS, Aviano (PN), Italy

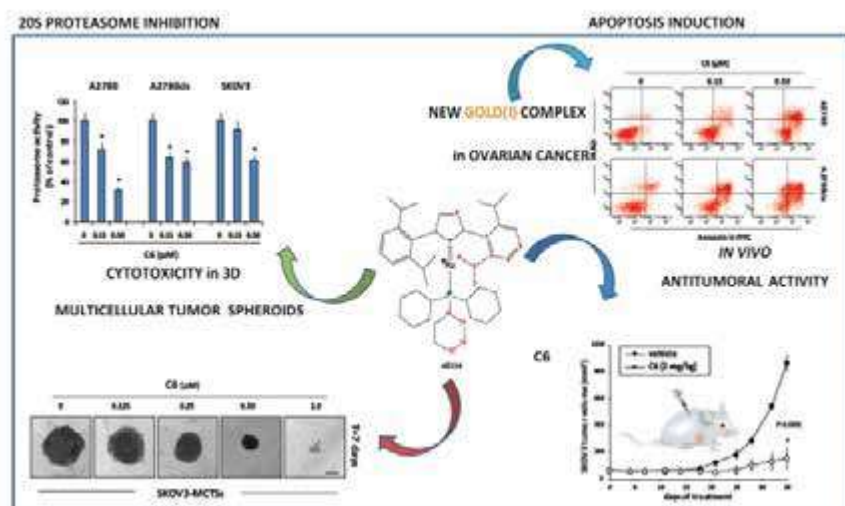
^cInterdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals,
 Dhahran 31261, Saudi Arabia

Corresponding author: adamahmed@kfupm.edu.sa

Abstract

A series of gold(I) complexes (1-7) incorporating 1,3-Bis(2,6-diisopropylphenyl)imidazol-2-ylidene (IPr) and phosphine ligands has been synthesized and assessed for antitumoral activity in ovarian cancer using in vitro and in vivo models. The synthesized complexes were characterized using elemental analysis, infrared spectroscopy, (¹H, ¹³C, and ³¹P) NMR spectroscopy, and X-ray diffraction crystallography. The antiproliferative efficacy of these novel complexes exceeded that of cisplatin in both cisplatin-sensitive (A2780) and cisplatin-resistant (A2780cis) ovarian cancer cells. The anticancer efficacy and mechanism of action of the most potent gold(I) complex 6 were further examined utilizing in vitro two-dimensional (2D) and three-dimensional multicellular tumor spheroid (MCTS) models of ovarian cancer, as well as in vivo tumor xenografts. Complex 6 triggered apoptosis, elevated mitochondrial reactive oxygen species production, and resulted in DNA damage (double strand breaks, DSBs) in A2780, A2780cis, and 3D-SKOV-3-MCTSs. Complex 6 inhibited the activity of the 20S proteasome, cell migration, and altered actin polymerization and distribution. Ultimately, Complex 6 demonstrated a substantial reduction in tumor growth of SKOV3-derived tumor xenografts without noticeable toxic side effects.

Keywords: Gold(I); carbene; phosphane; ovarian cancer; Multicellular spheroids



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SYNTHESIS AND CHARACTERIZATION OF BIS(IMINO)ACENAPHTHENE LIGANDS BEARING VARIOUS FLUOREDED SUBSTITUTION

Bilgehan Guzel^{a,*}, Burcu Tezcan^a, Elif Torun^a, Nora Ahmed^a

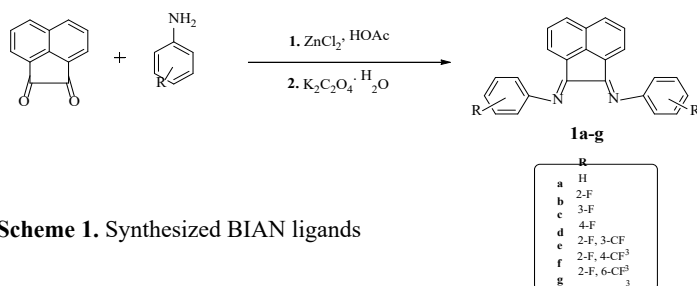
^a Department of Chemistry, Faculty of Arts and Science, Cukurova University, Adana, Turkey *Corresponding author: bilgehan@cu.edu.tr

Abstract

Bis(imino)acenaphthene (BIAN) ligands hold a significant position in the field of coordination chemistry due to their unique structure and reactivity. BIAN ligands possess strong σ -donating and good π -accepting properties, and these attributes enhance their effectiveness in catalytic applications¹. Due to their expanded pi system and rigid structures, their metal center wing angles become narrower, which improves control over the catalytic center². Extensive research in organic synthesis and materials science uses BIAN ligands to create new catalytic systems and advanced materials. Understanding their synthesis, properties, and applications is crucial for progress in coordination chemistry and exploring new opportunities in catalysis and material development. Particularly in organometallic chemistry, such salts play a significant role in enhancing the binding capabilities of transition metals. As a result, imidazolium salts can increase not only catalytic activity but also the selectivity and efficiency of reactions. Therefore, they find extensive use in chemical research and industrial applications.

In this study seven different diimine compounds with an acenaphthylene skeleton were synthesized using the ring-closing method, which is different from the traditional quaternization synthesis method. The characterization of the all-synthesized structures was analyzed using spectroscopic methods such as ¹H, ¹³C, ¹⁹F NMR, FTIR, elemental analysis, and HR-MS.

Keywords: *N*- Heterocyclic carbene, BIAN, diimine ligands, synthesis, characterization



Scheme 1. Synthesized BIAN ligands

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Acknowledgment

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CONTROLLABLE SYNTHESSES OF A TWO-DIMENSIONAL COORDINATION FRAMEWORK AND ITS DISCRETE HETEROLEPTIC BUILDING BLOCKS

Thanh Nhan Nguyen^a, Hyojong Yoo^{a*}

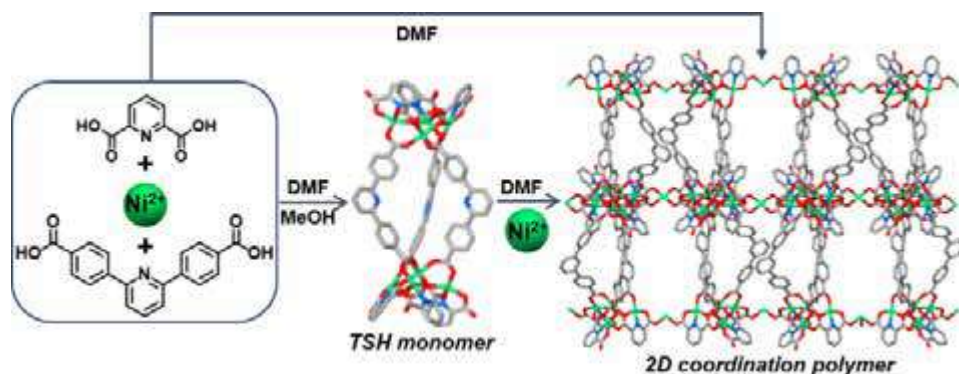
^a Department of Battery and Chemical Engineering, Hanyang University, Ansan, Gyeonggi-do 15588, Republic of Korea

*Corresponding author: hjhaha73@hanyang.ac.kr

Abstract

In supramolecular chemistry, creating self-assembled architectures with high functionality and complexity is highly desirable yet challenging. To achieve this purpose, recently, supramolecular chemists have utilized supermolecular building block (SBB) approach in which SBBs serve as direct building units to assemble metal-organic platforms. Since our first report on heteroleptic triple-stranded helicates (TSHs), in which two metal clusters (assembled from four transition metal ions and three 2,6-pyridinedicarboxylate ligands) are connected by three dicarboxylate bridging ligands, various discrete coordination cages (0D) or 1D polymers have been reported. However, to date, 2D polymers constructed from TSH building blocks have yet to be reported. Herein, controllable syntheses of a two-dimensional (2D) coordination polymer and its discrete triple-stranded helicate (TSH) building units using a solvent-assisted approach are reported. Each single TSH is assembled from two multinuclear nickel clusters interconnected by three V-shaped 4,4'-pyridine-2,6-diylidibenzoate (PDDB) bridging ligands. The long distance between two terminal carboxyl groups, together with the bending angle of 120° in the PDDB, generates a void inside the TSH, which is functionalized by the pyridinic ring at the center of PDDBs. Dimethylammonium ions, which are present in the solid state of discrete TSHs, neutralize the charge of TSHs and stabilize the solid structure with hydrogen bonding. Large-sized TSHs possess high connectivity and proper symmetry, making them suitable for constructing a 2D hierarchical coordination framework—a rare coordination platform obtained via the supermolecular building block (SBB) approach. The conversion of discrete TSHs into a 2D framework demonstrates their suitability as SBBs for constructing higher-order coordination-driven frameworks.¹

Keywords: Supermolecular building block (SBB), coordination polymer, functionalized cavity, 4,4'-pyridine-2,6-diylidibenzoate ligand, solvent-assisted synthesis



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TAILORING CALCIUM CONTENT AND BIOACTIVITY IN SiO₂-CaO MESOPOROUS BIOACTIVE GLASS NANOPARTICLES FOR BONE TISSUE ENGINEERING

Ekarat Meechoowas^{a*}, Usanee Pantulap^a, Phitsamai Kamonpha^a, Pakchanok Sueakong^a, Siwaporn Sirilaksattha^a, Savarin Sinaviwat^a, Sureerat Yodthuan^a, Nuttawan Sawangboon^a

^a*National Institute of Reference Laboratories, Department of Science Service, Bangkok, Thailand*

^{*}*Corresponding author: ekarat@dss.go.th*

Abstract

Mesoporous bioactive glass nanoparticles (MBGNs) based on the SiO₂-CaO binary system show considerable potential for biomedical applications due to their highly ordered mesoporous structures, nanoscale dimensions and large specific surface area. Recently, MBGNs have gained significant attention in implant technologies, including coatings for metallic implants, scaffold composites, and bone cement formulations. However, calcium oxide (CaO) incorporation remains limited (about 15 mol%) with conventional synthesis methods, especially the classic Stöber procedure that uses tetraethyl orthosilicate (TEOS) and calcium nitrate (Ca(NO₃)₂). Increasing CaO content beyond this limit is crucial, as it significantly improves bioactivity, osteoconductivity, and the regenerative potential. In this study, the impact of two different calcium precursors (calcium nitrate and calcium hydroxide (Ca(OH)₂)) was systematically investigated using a modified Stöber synthesis, aiming to enhance the CaO content in MBGNs. Comprehensive characterization was performed, including scanning electron microscopy (SEM), elemental analysis (EDS), X-ray fluorescence (XRF) spectroscopy, nitrogen adsorption-desorption analysis, and bioactivity assessment in simulated body fluid (SBF). XRF and EDS results demonstrated a substantial increase in CaO content, approximately double when Ca(OH)₂ was used compared to Ca(NO₃)₂-derived nanoparticles. MBGNs synthesized using Ca(OH)₂ revealed consistent spherical-to-oval morphology, with particle diameters ranging between 200–300 nm, and exhibited enhanced textural properties, notably increased pore volume and surface area. Additionally, bioactivity studies confirmed rapid formation of hydroxyapatite-carbonate layers on these nanoparticles during SBF immersion, further emphasizing the improved osteogenic potential. Overall, these findings highlight the critical role of calcium precursor selection on tailoring the physicochemical characteristics and bioactivity of MBGNs, underscoring their potential as advanced bone fillers and scaffolds for regenerative medicine.

Keywords:

mesoporous bioactive glass, calcium precursors, bioactivity, nanoparticles, modified stöber method

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SOL-GEL-DERIVED BIOACTIVE GLASS AS A REFERENCE STANDARD FOR IN VITRO APATITE FORMATION: A COMPARISON WITH MELT-QUENCH GLASS

Usanee Pantulap^{a,*}, Nuttawan Sawangboon ^a, Kansiree Kaewmorakot^a,
Surirat Yotthuan^a, Phitsami Kamonpha^a

^a National Institute of Reference Laboratories,
Department of Science Service, Thailand

*Corresponding author: usanee@dss.go.th

Abstract

In vitro studies using simulated body fluid (SBF) are widely employed to evaluate the bioactivity of materials through the formation of a hydroxyapatite (HA) layer on their surfaces. SBF mimics the ion concentrations of human blood plasma, and HA formation is a key indicator of bone-bonding potential. To ensure the validity of SBF preparation, ISO/FDIS 23317 recommends the use of standard glasses with known HA-forming ability. This study aims to fabricate bioactive glass standards via sol-gel processing and investigate their potential as alternative reference materials to conventional melt-quench-derived glass. The Sol-gel glass and melt-quench glass were synthesized and characterized for chemical composition (X-ray fluorescence, XRF), phase purity (X-ray diffraction, XRD), and morphology (scanning electron microscopy, SEM). Upon immersion in SBF for 12, 24, and 120 hours, the HA-forming ability of both materials was evaluated using XRD and SEM. The sol-gel-derived glasses demonstrated finer particle size, greater surface area, and a significantly faster HA nucleation rate than the melt-quench-derived glasses. These findings highlight the potential of sol-gel-derived bioactive glass as a more responsive and effective standard for in vitro bioactivity testing.

Keywords: sol-gel method, hydroxyapatite formation, in vitro bioactivity, glass standard, ISO/FDIS 23317

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THE CHEMISTRY OF 10-VERTEX ELECTRON-RICH CARBORANE CLUSTERS

Vlastimil Němec^{a,*}, Jan Vrána^a, Josef Holub^b, Maksim A. Samsonov^a, Aleš Růžička^a

^aDepartment of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, 532 10 Pardubice, Czech Republic

^bInstitute of Inorganic Chemistry, Czech Academy of Sciences, 250 68 Řež, Czech Republic

*Corresponding author: st60099@student.upce.cz

Abstract

The polyhedral boranes and heteroboranes appear almost exclusively in neutral or anionic forms, while the cationic bear the positive charge at exoskeletal heteroatoms or they are instable at room temperature. In 2021, we described the first thermally robust cationic carboranes supported by bulky N-heterocyclic carbenes. Due to a strong σ -donation to carboranes, the polarity is reversed, and the clusters accept the proton from acids to yield cationic clusters. In this work, the reactivity of 10-vertex closo-dicarba-boranes with different N-heterocyclic or mesoionic carbenes will be presented as along with the structural rearrangements of the carbene-carborane complexes to thermodynamically stable products. The reactivity of such electron-rich clusters with various acids, transition metal complexes, and main group compounds will be discussed as well.

Keywords: main-group chemistry, 10-vertex carboranes, N-heterocyclic carbene, mesoionic carbene, coordination chemistry.

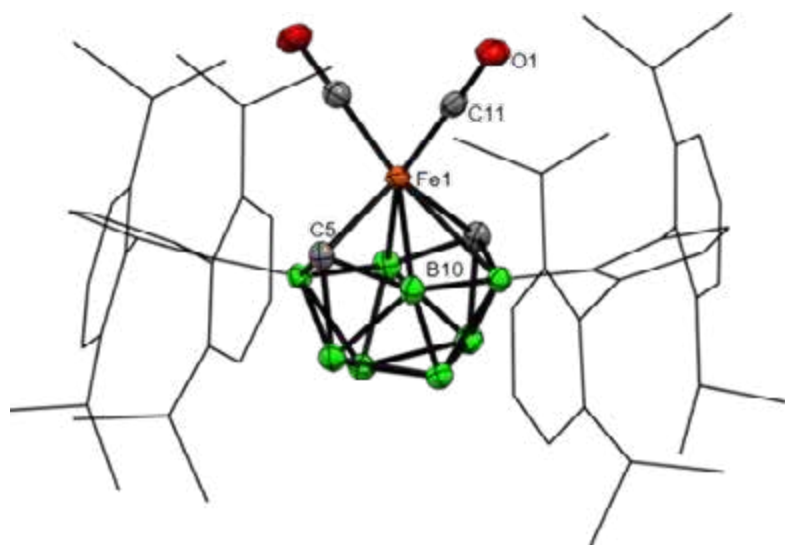


Figure 1 The molecular structure of [closo-(2,6-NHC^{Dipp}-1,10-C₂B₈H₈)Fe(CO)₂]

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SYNTHESIS, STRUCTURAL CHARACTERIZATION, AND CATALYTIC PERFORMANCE OF Pd(II) COMPLEXES WITH FLUORINE- AND METHYL-SUBSTITUTED SCHIFF BASES: EXPERIMENTAL AND THEORETICAL INSIGHTS

Nur Husnina Nasaruddin^a, Shahrul Nizam Ahmad^{a,*}, Amalina Mohd Tajuddin^{a,c},
Nova Pratiwi Indriyani^d, Aditya Wibawa Sakti^e, Yessi Permana^d, Nor Mas Mira Abd Rahman^b,
Nor Saadah Mohd Yusof^b, Hadariah Bahron^a

^aFaculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia

^bDepartment of Chemistry, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia

^cAtta-ur-Rahman Institute for Natural Product Discovery (AuRIns), UiTM Kampus Puncak Alam, 42300 Bandar Puncak Alam, Selangor, Malaysia

^dInorganic and Physical Chemistry Research Division, Institut Teknologi Bandung, Jl. Ganesha 10, Bandung 40132, Indonesia

^eDepartment of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Tokyo 169-8555, Japan

*Corresponding author: shahruln@uitm.edu.my

Abstract

Two meta-substituted Schiff bases were synthesized and characterized using physicochemical and spectroscopic analysis. These Schiff bases were complexed with palladium(II) to form [Pd(AD1F)] and [Pd(AD1Me)], both characterized through single-crystal X-ray diffraction, elemental analysis, molar conductivity, FTIR, ¹H NMR, and UV-Vis spectroscopy. Pd(AD1F) crystallized in a monoclinic system (P21/c space group), with the phenolic oxygen and azomethine nitrogen chelating Pd(II) to form a distorted square planar geometry. The complexation of the ligand to Pd(II) through the azomethine nitrogen was confirmed from the IR blue shift and the shift of azomethine proton resonances to higher or lower chemical shifts in ¹H NMR. Additionally, the shift of the n-π*(C=N) band in UV-Vis spectra indicated the involvement of azomethine nitrogen in the complexation. Pd(AD1Me) has been previously reported in our earlier work. DFT calculations revealed similar electronic transitions at 259 nm (π → π*) and 333 nm (n → π*), dominated by specific HOMO to LUMO transitions for [Pd(AD1Me)] and [Pd(AD1F)] with minor effects from substituents. [Pd(AD1F)] demonstrated catalytic activity in copper-free Sonogashira coupling, achieving a TOF of 2.4h⁻¹ and a TON of 7.1 at 120 °C. Its higher ionization potential and lower electron affinity, as determined by DFT, supporting its superior catalytic performance compared to [Pd(AD1Me)].

Keywords: Schiff base, Palladium, Sonogashira, DFT, Single crystal

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SYNTHESIS OF ZSM-5 ZEOLITE FROM PADMA RIVER SAND AS AN ALTERNATIVE SOURCE OF SILICA

Aparna Sarker^a, Robayath Jahan Rabeya^a, Nasrin Akter Nadi^a, A.K.M. Lutfur Rahman^{a*},

^aDepartment of Chemistry, Jagannath University, Dhaka, Bangladesh

*Corresponding author: lrahman@chem.jnu.ac.bd

Abstract

Zeolites, particularly ZSM-5, are widely used in catalytic and environmental applications due to their unique properties. This study investigates the synthesis of ZSM-5 zeolite using silica extracted from Padma River sand in Munshigonj, Bangladesh, a cost-effective alternative for catalyst production. High-purity amorphous silicon dioxide (SiO₂) was successfully extracted from sand, as confirmed by X-ray diffraction (XRD) analysis and utilized in a hydrothermal synthesis method. The optimal synthesis conditions for ZSM-5 included a temperature of 150°C, reaction time of 48 hours, and a SiO₂/Al₂O₃ molar ratio of 54. These parameters yielded well-crystallized ZSM-5 with tetrapropyleammonium bromide (TPABr) acting as the structure-directing agent. The synthesized zeolite was characterized using XRD, FTIR, SEM, and XRF, which confirmed the MFI phase (characteristic of ZSM-5), a pentasil framework structure with polycrystalline spherical morphology. Notably, lower SiO₂/Al₂O₃ ratios produced poorly crystalline or amorphous zeolite, whereas the optimal ratio (54) resulted in highly ordered crystals. Additionally, the ZSM-5 zeolite demonstrated significant antimicrobial activity with antibacterial effects against *Salmonella paratyphi* and *Shigella dysenteriae*, and antifungal activity against *Aspergillus flavus* and *Trichoderma harzianum*. This study underscores the potential of locally sourced silica (Padma river sand) for synthesizing ZSM-5 with applications in catalysis and antimicrobial treatments.

Keywords: ZSM-5, hydrothermal synthesis, silica from Padma river sand.

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HYDROPHOBIC MODIFICATION OF SBA-15 WITH ENCAPSULATED In_2O_3 CATALYST: ENHANCED CO_2 -TO-METHANOL CONVERSION EFFICIENCY

Heng Zhang^a, Dongfang, Wu^{a*}

^a Department of Chemical Engineering, School of Chemistry and Chemical Engineering, Southeast University, Jiangning District, Nanjing 211189, China.

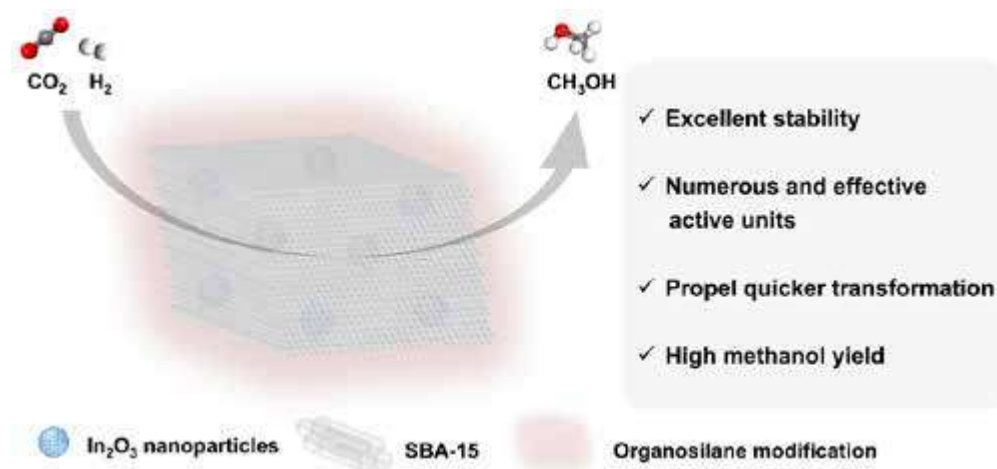
*Corresponding author: dfwu@seu.edu.cn

Abstract

Stable and efficient heterogeneous catalysts are crucial for commercial CO_2 hydrogenation to methanol. Currently, In_2O_3 has attracted much attention because of its surface oxygen vacancy, which can promote the conversion of CO_2 to methanol.¹ However, the limited active sites only in the surface phase and the poor stability of In_2O_3 -based catalysts confines their application prospect, making it far from being the answer to the problem of slow methanol synthesis efficiency.^{2,3} Herein, we prepared a catalyst using the in-situ hydrothermal method, in which In_2O_3 nanoparticles were encapsulated in the SBA-15 molecular sieve, followed by hydrophobic modification. The results show that the In_2O_3 component is separated into small nanoparticles in SBA-15, and they could be used as active units for the CO_2 hydrogenation reaction. Moreover, the excellent specific surface area and abundant mesopores of SBA-15 can promote more CO_2 to undergo hydrogenation in the In_2O_3 active unit, thereby achieving higher methanol synthesis efficiency. Furthermore, the hydrophobic modification of the catalyst can facilitate the rapid desorption of water (one of the reaction products), thus promoting the rapid operation of the reaction and greatly improving the methanol yield. On the other hand, it also avoids the structural damage caused by the adsorption of water on the surface structure of In_2O_3 , so that the stability of the catalyst is greatly improved. This work highlights the importance of targeted design and performance modulation of catalysts in advancing catalyst development and applications.

Keywords: heterogeneous catalyst, hydrophobic modification, encapsulation, CO_2 hydrogenation, methanol synthesis

Graphic / Image



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EXPLORING NOVEL ZINC COMPLEXES WITH PICOLINATO DERIVATIVES: SYNTHESIS AND ANALYSIS

M. Hozjan^{a*}, F. Perdih^a,

^a Faculty of Chemistry and Chemical Technology, University of Ljubljana

*Corresponding author: misel.hozjan@fkkt.uni-lj.si

Abstract

The escalating prevalence of diabetes mellitus in the 21st century highlights the need for novel therapeutic strategies. Certain metal ions, including zinc(II), have demonstrated antidiabetic effects, with zinc being particularly significant due to its involvement in numerous biological processes.¹ However, the bioavailability and efficacy of Zn(II) are critically dependent on its chemical form.² Complexation with organic ligands offers a powerful approach to modulate these properties and enhance its therapeutic potential.

Inspired by the promising antidiabetic activity observed in previous coordination compounds with picolinato ligands,^{3,4} we designed and synthesized a library of novel picolinic acid derivatives. Starting from pyridine-2,6-dicarboxylic acid, we introduced amine functional groups to prepare a set of ligands. These derivatives were subsequently complexed with zinc(II) ions, and the resulting materials were characterized. Solution studies were conducted to elucidate the behaviour of these complexes in relevant media. Furthermore, the synthesized compounds were evaluated in biological assays to assess their biological activity.

Single-crystal X-ray diffraction of the obtained crystals revealed a variety of coordination modes adopted by the zinc(II) center, highlighting the influence of the ligand structure, pH, and zinc precursor on the final complex architecture. An example of an obtained structure is shown on Figure 1.

Keywords: picolinic acid, zinc, crystallography, coordination chemistry, diabetes

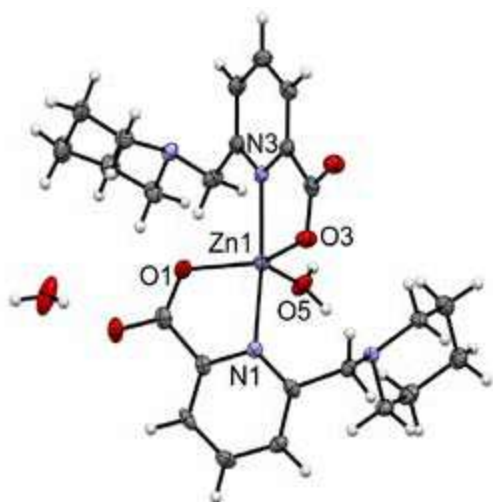


Figure 1: An example of a prepared Zn(II) complex with 6-(piperidin-1-ylmethyl)picolinic acid.

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PROCESSING OF METAL-ORGANIC FRAMEWORKS FOR ARSENIC REMOVAL FROM PETROLEUM PRODUCTS

Phakawan Thinsoongnoen^a, Kunlanat Sriphumrat^a, Kanokwan Kongpatpanich^{a,*}

^aDepartment of Materials Science and Engineering, School of Molecular Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Rayong, 21210, THAILAND

*Corresponding author: kanokwan.k@vistec.ac.th

Abstract

Arsenic contamination in petroleum products significantly impacts the oil and gas industry due to catalyst poisoning and subsequent operational disruptions in downstream refining processes. While extensive research has been conducted on arsenic removal in aqueous environments, research on arsenic removal in petroleum-based matrices remains limited. To address this challenge, a one-pot synthesis has been developed to produce a gel-like UiO-66 metal-organic framework (MOF) optimal rheological properties suitable for binder-free pelletization, while maintaining high surface area and defect-rich active sites essential for arsenic adsorption. The resulting MOF pellets exhibited high arsenic adsorption capacities for both As(III) and As(V), achieving over 90% removal efficiency in natural gas condensates with excellent durability over 20 adsorption-desorption cycles. To further improve removal efficiency and broaden the scope of application, an amino-functionalized Zr-based MOF has been developed, featuring dual accessible binding sites derived from structural defects at Zr clusters and ligand functional groups on the ligands. This MOF demonstrates exceptional dual adsorption capacities for both As(III) and Hg(II). Comprehensive mechanistic studies indicated that metal cluster defect sites are the primary adsorption sites, while functionalized amino groups stabilize the MOF structure and enhance adsorption performance. The works propose the importance of MOF design strategies for effectively addressing arsenic and mercury contamination in challenging hydrocarbon and environmental systems.

Keywords: Metal-organic frameworks, Adsorbent, Arsenic, Petroleum contaminant, Wastewater

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CHELATING “CARBONE” LIGANDS: SYNTHESIS, METAL COORDINATION AND REACTIVITY STUDY

Bamlaku Semagne Aweke,^[a] Wen-Ching Chen,^[a] Glenn. P.A. Yap,^[d] Lili Zhao^{*[b]} and Tiow-Gan Ong^{*[a,c]}

^aInstitute of Chemistry, Academia Sinica, Taipei, Taiwan

^bInstitute of Advanced Synthesis, School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing, China

^cDepartment of Chemistry, National Taiwan University, Taipei, Taiwan

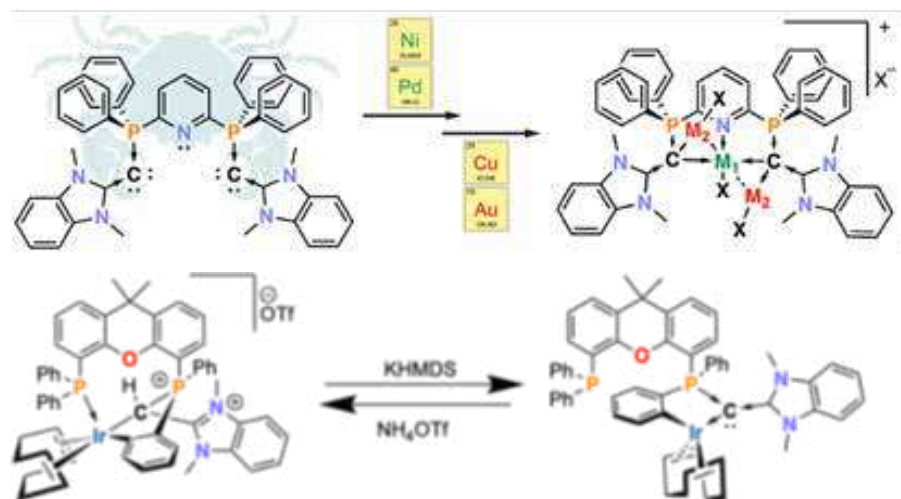
^dDepartment of Chemistry and Biochemistry, University of Delaware, Newark, USA

*Corresponding author: tgong@gate.sinica.edu.tw

Abstract

Carbones are divalent carbon(0) species featuring two lone pairs of electrons, which grant them a distinctive flexibility in coordination with metals. This unique attribute allows carbone ligands to simultaneously engage both electron pairs, a property often exploited to isolate geminal bimetallic complexes. In this study, we report the synthesis of chelating carbone ligands, including the first stable and isolable free bis(carbone) pincer framework, using a novel synthetic approach. We further explored their coordination behavior with various transition metals. These ligands, characterized by well-defined solid-state structures, serve as effective scaffolds for coordination both monometallic and heteronuclear trimetallic complexes, such as Au–Pd–Au, Au–Ni–Au, and Cu–Ni–Cu. Advanced quantum-chemical analyses revealed that the metal–metal interactions within these complexes are relatively weak and do not significantly contribute to their structural integrity. Instead, the stability of these multi-metallic architectures primarily arises from the four lone pairs of electrons residing in the bis(carbone) framework. Moreover, we demonstrated the unique reactivity of an Ir(I) complex bearing a carbone ligand, which undergoes reversible and controlled intramolecular coordination–decoordination. Additionally, we observed notable small-molecule activation behavior in a Pd(II) complex supported by this chelating carbone ligand.

Keywords: Carbone, Chelating ligand, bis(carbone)



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MECHANISTIC STUDY OF NICKEL-CATALYZED CARBON-OXYGEN BONDS ARYLATION REACTION OF HETEROARYL ETHERS

Chen-Hsun Hung^{b,‡}, Ting-Hsuan Wang^{a,*‡}, Jiun-Shian Shen^{b,c,‡}, Manman Zhud, Jia-Huei Luoh^b,
 Bamlaku Semagne Awekeb^c, Jie-Ting Fub, Sin-Yu Chen^b, Yin-Zhi Weng^{b,c}, Chih-Wen Paoe,
 Glenn P. A. Yapf, Ping-Yu Cheng^{*}, Lili Zhaod^{*} and Tiow-Gan Ong^{b,c,*}

^a Hubei Key Laboratory of Processing and Application of Catalytic Materials, Huanggang Normal University, Huanggang (China).

^b Institute of Chemistry, Academia Sinica, Taipei (Taiwan)

^c Dept. of Chemistry, National Taiwan University, Taipei (Taiwan)

^d State Key Laboratory of Materials-Oriented Chemical Engineering, School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing (China)

^e National Synchrotron Radiation Research Center, Hsinchu (Taiwan)

^f Dept. of Chemistry and Biochemistry, University of Delaware Newark, DE (USA)

^g Dept. of Chemistry, National Chung Hsing University, Taichung (Taiwan)

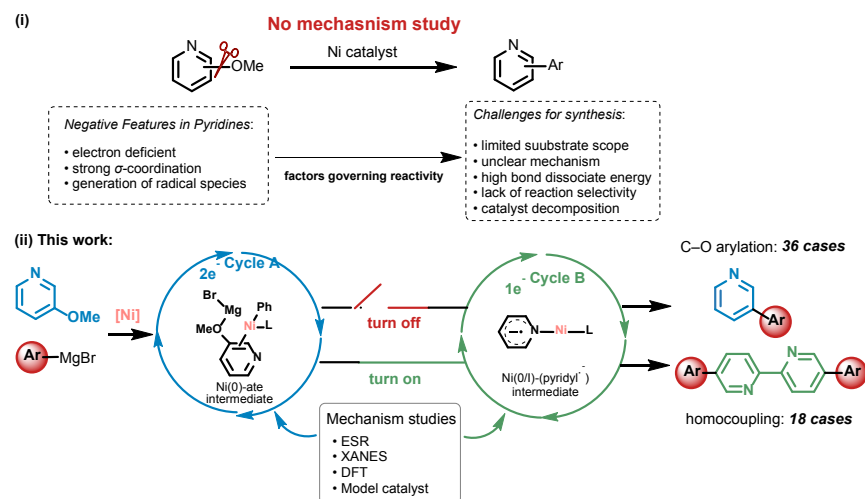
[‡] These authors contributed equally.

*Corresponding author: tgong@gate.sinica.edu.tw; tinawang7747@hgnu.edu.cn, pychen@dragon.nchu.edu.tw, ias_llzhao@njtech.edu.cn

Abstract

The C–O bond activation in aryl ether derivatives offers a greener route by avoiding the need for halogenated electrophiles. In this work, we report detailed mechanistic analysis concerning the nickel mediated C–O transformation of pyridyl methyl ethers. Supported by DFT calculation, X-ray absorption spectroscopy (XAS), electron spin resonance (ESR) and model catalyst, two distinct catalytic cycles were elucidated (i) the cycle A, responsible for C–O arylation via on a Ni(0)/Ni(II) redox manifold and (ii) the cycle B, involving key Ni(0/I)-pyridine radical cage species that promotes pyridine-pyridine homocoupling. These mechanistic insights were applied to substrate scope studies, allowing switchable catalysis for selective pyridine arylation and bipyridine synthesis.

Keywords: C–O arylation • metal–ligand redox cooperativity • nickel • pyridine • heterocycles



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MACHINE LEARNING-GUIDED MONODENTATE LIGAND MAP WITH ELECTRONIC AND STERIC FEATURES AND ITS APPLICATION IN CATALYSIS

Chen-Hsun Hung^a, and Tiow-Gan Ong^{a,b*}

^a*Institute of Chemistry, Academia Sinica, Taipei, Taiwan.*

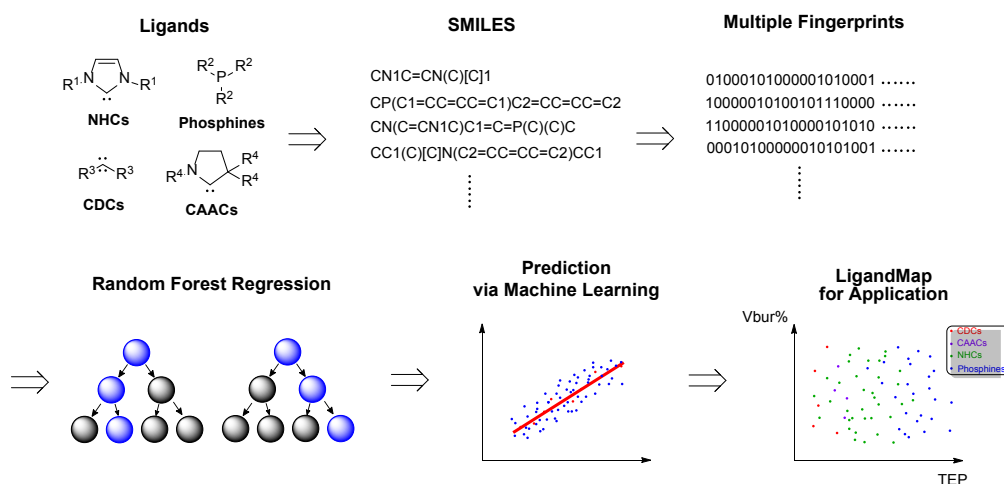
^b*Department of Chemistry, National Taiwan University, Taipei, Taiwan.*

^{*}*Corresponding author: tgong@gate.sinica.edu.tw*

Abstract

The electronic and steric properties of ligands are two important features which show enormous effects in catalytic reactions.¹⁻² Herein, we reported a map about electronic and steric factors of various monodentate ligands, including common phosphines, NHCs, CAACs, and CDCs. The ligand map is constructed via machine learning prediction, which converts ligands into digits with structure-based multiple fingerprints³ and is predicted with random forest regression algorithm. A 3D plot of the yields in catalytic reaction with this map could further give us another perspective to understand the relationship between yields and the electronic/steric factors of ligands.⁴⁻⁵

Keywords: ligand, Tolman electron parameter, buried volume, machine learning



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SYNTHESIS AND CHARACTERIZATION OF CHIRAL BINAP-CARBONE METAL COMPLEXES AND THEIR APPLICATION IN CATALYSIS

Ying-Yu Chen,^{a,b} He-Xin Xiao,^{b,d} Ching-Yu Liao,^c Wen-Ching Chen,^b Glenn P. A. Yap^e and Tiow-Gan Ong^{b,d*}

^a National Taiwan University of Science and Technology, Taipei, Taiwan (R.O.C)

^b Institute of Chemistry, Academia Sinica, Taipei, Taiwan (R.O.C)

^c Department of Chemistry, National Central University, Taoyuan, Taiwan (R.O.C)

^d Department of Chemistry, National Taiwan University, Taipei, Taiwan (R.O.C)

^e The Department of Chemistry and Biochemistry, University of Delaware, Newark, DE (USA)

*Corresponding author: tgong@gate.sinica.edu.tw

Abstract

Carbophosphinocarbenes (CPCs) possess two lone pairs of electrons available for donation towards transition metals.¹ We have successfully synthesized the racemic BINAP-CPC and its precursor, the bent salt, which were employed as ligands to form palladium and bimetallic copper complexes. The solid-state structures of these complexes were thoroughly characterized using single crystal X-ray diffraction. In the case of BINAP-CPC Pd(II) complexes, they were utilized in Suzuki-Miyaura cross-coupling reactions. Due to the significant difference in donor strength between the bent salt and CPC ligand, we anticipate that chemo-selectivity would be evident when examining a substrate with multiple functional groups, such as 4-bromophenyl-trifluoromethanesulfonate. Consequently, experimental observations clearly demonstrated that the Csp²-Br bond reacted prior to the Csp²-OTf bond, resulting in the formation of the mono-cross-coupling major product.² On the other hand, BINAP-CPC Cu complexes were employed as bimetallic catalysts in the hydroboration of internal and terminal alkynes with Bis(pinacolato)diboron (B₂pin₂), yielding moderate to good reactivity (Figure 1).

Keywords: Binap, Transition metals, Suzuki-Miyaura reaction, Hydroboration, Racemic compound

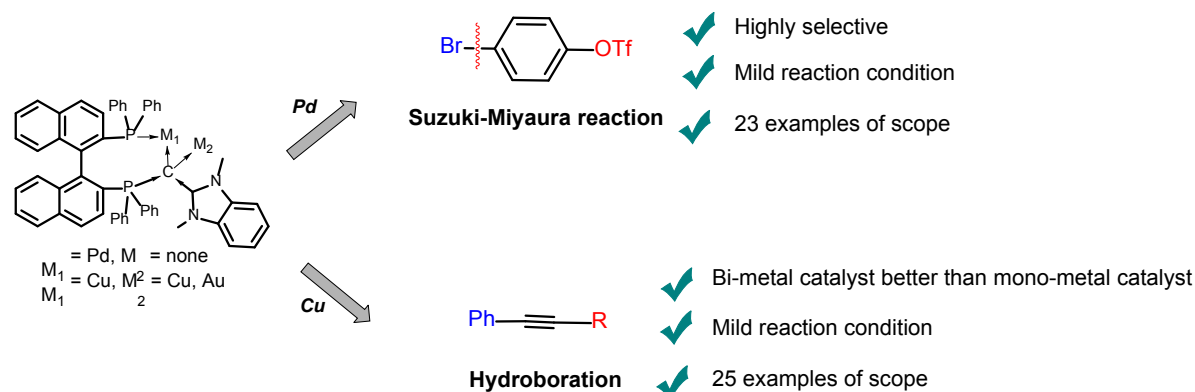


Figure1. Synthesis of BINAP-carbone metal complexes and their application in Suzuki-Mayaura and hydroboration reaction

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ISOLATED CARBON(I) SPECIES FEATURING A CARBONE CATION RADICAL

He-Xin Xiao^{a,b}, Yi-Chen Chan^a, Lei Qin^c, Yun-Wei Chiang^{*d}, Gernot Frenking^{*e}, Lili Zhao^{*d},
Tiow-Gan Ong^{*a,b},

^a*Institute of Chemistry, Academia Sinica, Taipei, Taiwan, R.O.C.*

^b*Department of Chemistry, National Taiwan University, Taipei, Taiwan, R.O.C.*

^c*State Key Laboratory of Materials-Oriented Chemical Engineering, School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing, China.*

^d*Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, R.O.C.*

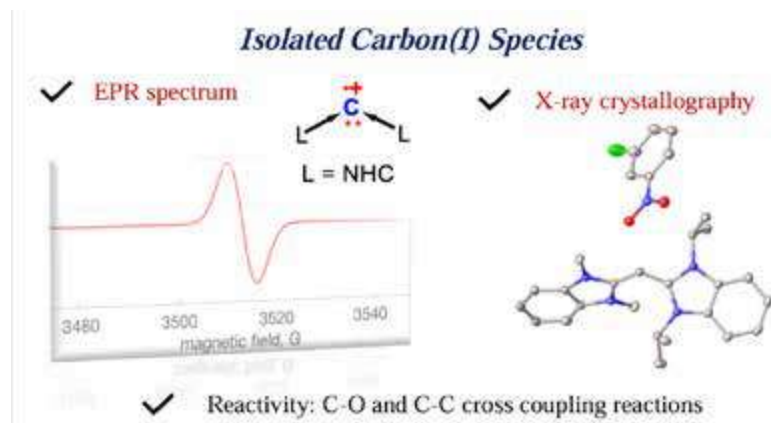
^e*Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Strasse, D-35043 Marburg, Germany*

^{*}*Corresponding author: tgong@gate.sinica.edu.tw*

Abstract

Carbynes, characterized by their radical and carbene attributes, possess three nonbonding electrons and have garnered significant scientific interest. The high reactivity and complex hybridization of valence orbitals in carbynes have impeded the isolation of free carbon(I) species. Carbodicarbenes are divalent carbon (0) species with two electron lone-pairs^{1,2}, which are in principle capable of losing an electron to generate a radical cation carbon(I) species containing three non-bonded electrons, similar to the frontier orbital of a carbyne without a vacant orbital. Herein, we describe the isolation of a crystalline cation radical carbon(I), $[1\text{-CDC}]^{+\bullet}$, prepared by a single electron transfer (SET) between a carbodicarbene and a nitro aromatic compound to generate a stable radical ionic pair. Electron paramagnetic resonance (EPR) and X-ray crystallography with quantum chemical analysis show that the unpaired electron of $[1\text{-CDC}]^{+\bullet}$ resides in the $p(\pi)$ atomic orbital (AO) of the secondary carbon with some delocalization to the N-heterocyclic carbene (NHC) ligands. Exploring the reactivity of this carbon(I) radical cation revealed its capacity to mediate a variety of C-O and C-C cross coupling reactions with electron-deficient aryl halides. These findings not only expand the understanding of carbon(I) radical chemistry but also open new avenues for radical methodologies in organic synthesis and catalysis.

Keywords: carbene; radical cation, Carbon(I), bonding analysis



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A VERSATILE CARBODICARBENE PRECURSOR: EXPLORING COORDINATION AND REACTIVITY WITH TRANSITION METALS AND MAIN GROUP ELEMENTS

Zhe-Xin Wu^{a,b}, Jiun-Shian Shen^{b,c}, Glenn P. A. Yap^d, Tiow-Gan Ong^{b,c*}

^a Department of Chemistry, National Central University, Taoyuan, Taiwan (R.O.C)

^b Institute of Chemistry, Academia Sinica, Taipei, Taiwan (R.O.C)

^c Department of Chemistry, National Taiwan University, Taipei, Taiwan (R.O.C)

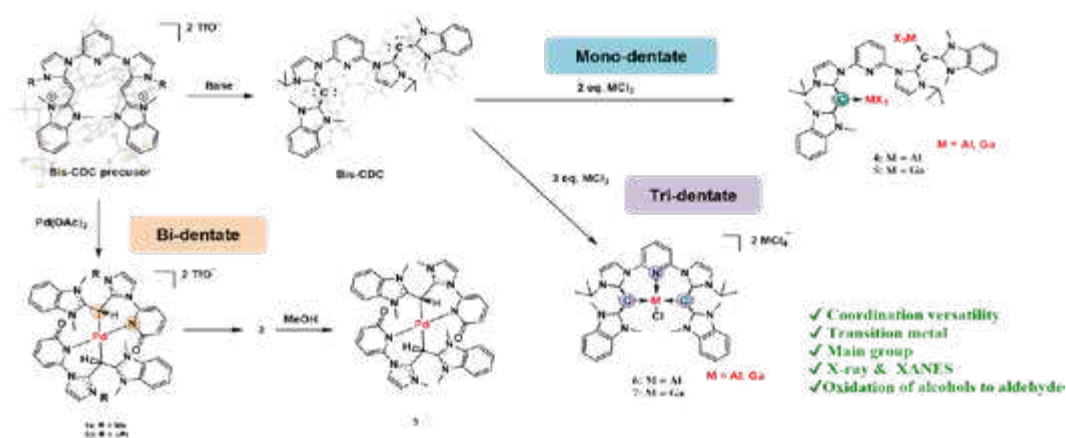
^d The Department of Chemistry and Biochemistry, University of Delaware, Newark, DE (USA)

*Corresponding author: tgong@gate.sinica.edu.tw

Abstract

Carbones, divalent carbon(0) species with two lone pairs of electrons, have emerged as highly electron-rich ligands capable of coordinating with both transition metals and main-group elements¹. Among them, carbodiphosphoranes (CDPs), carbodicarbenes (CDCs), and carbophosphinocarbenes (CPCs) have represent versatile ligand frameworks. The stable and isolable free bis-(carbone) pincer framework was first developed in our lab². Herein, we report the synthesis of the first bis-carbodicarbene (bis-CDC) ligand, designed to explore its coordination versatility and electronic behavior. The bis-CDC ligand and its metal complexes were synthesized and structurally characterized. Single-crystal X-ray diffraction revealed a bidentate coordination mode in **Pd(II)** complexes, and a tridentate binding mode in main-group metal complexes, including **Al(III)** and **Ga(III)**. X-ray absorption spectroscopy (XAS), including X-ray absorption near-edge structure (XANES), was employed to probe the electronic structures and oxidation states of complexes (1, 2 and 3), highlighting the non-innocent behavior of the CDC ligand. Furthermore, the complex 2 exhibited catalytic activity in the oxidation of alcohols to aldehydes. In conclusion, the bis-CDC ligand exhibits diverse coordination modes and promising reactivity with both transition and main-group metals. These findings broaden the application scope of CDC-based frameworks in coordination chemistry, catalysis, and materials science.

Keywords: Carbodicarbene, chelating ligand, bis(carbone), transition metal, main group elements



Scheme 1. Synthesis of bis-CDC and its Pd(II) and Al(III), Ga(III) complexes.

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COUPLING WITH HETEROARENE AND ARENOL VIA NI-CATALYZED C–H/C–OH ACTIVATION

Chen-Hsun Hung,^a Sin-Yu Chen,^{a,b} Ting-Hsuan Wang,^d and Tiow-Gan Ong ^{a,c*}

^aInstitute of Chemistry, Academia Sinica, Taipei, Taiwan

^bDepartment of Chemical Engineering, Nation Taiwan University of Science and Technology Taipei, Taiwan

^cDepartment of Chemistry, National Taiwan University, Taipei, Taiwan

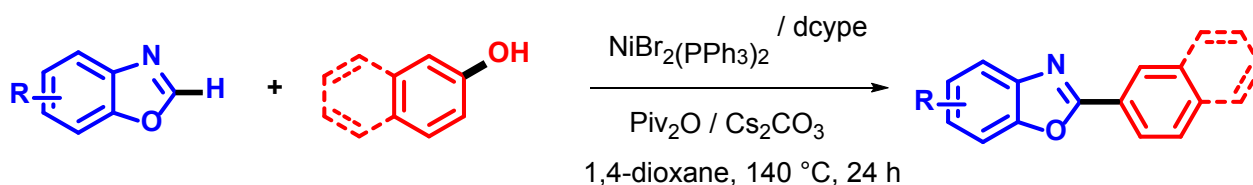
^dSchool of Chemistry and Chemical Engineering, Huanggang Normal University, Huanggang, Hubei, P. R. China

*Corresponding author: *tgong@gate.sinica.edu.tw

Abstract

Activation of arenols via C–O bond activation as coupling partner has been established with Ni-catalyzed cross-coupling with heteroarenes. With characterization of several Ni(II) complexes, monitoring reactions with NMR spectroscopy, KIE experiments, and kinetic studies, we proposed that oxidative addition occurred with Ni catalyst and pivalate-protected arenol derivatives via C–O bond activation, which was followed by base-assisted C–H activation of heteroarene and reductive elimination to form coupling product. This Ni/dcype system gave an alternative route to activate arenols via protection in one-pot reaction.

Keywords: Ni-catalyzed cross-coupling, C–H activation, C–O cleavage, in situ activation



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PALLADIUM AND IRIDIUM – CARBODICARBENE COMPLEXES FORMATION AND UNEXPECTED REACTION SELECTIVITIES

Min-Xuan Zhang^{a,b}, Jiun-Shian Shen^{a,c}, Zhe-Xin Wu^{a,b}, Wen-Ching Chen^a,
 Chen-Hsun Hung^a, Glenn P. A. Yap^d, Tiow-Gan Ong^{*a,c}

^aInstitute of Chemistry, Academia Sinica, Taipei, Taiwan

^bDepartment of Chemistry, National Central University, Taoyuan, Taiwan

^cDepartment of Chemistry, National Taiwan University, Taipei, Taiwan

^dDepartment of Chemistry & Biochemistry, University of Delaware, Newark, DE, USA

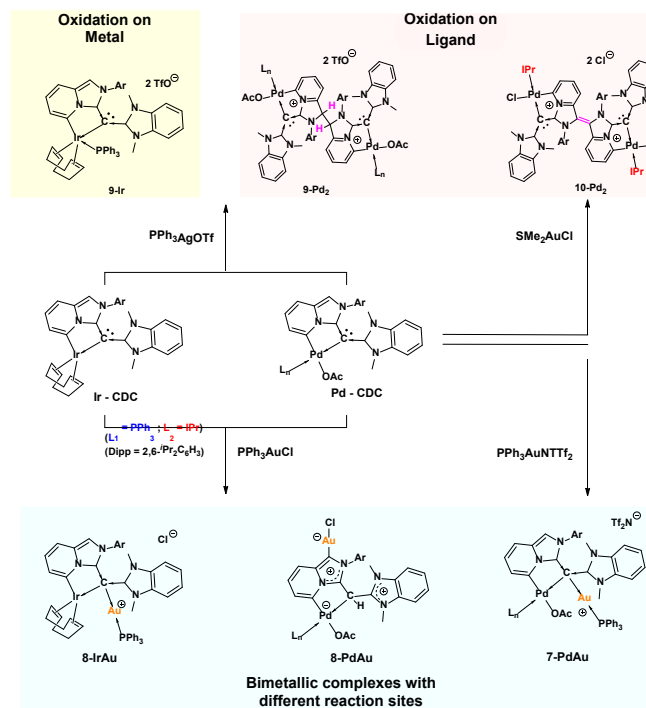
*Corresponding author: tgong@gate.sinica.edu.tw

Abstract

The Carbodicarbene (CDC) features¹⁻² two lone pairs of electrons at its zero-valent carbon center C(0), exhibiting both σ - and π -donating abilities. Using imidazo[1,5-a]pyridine as the scaffold for CDC, we synthesized monometallic Pd and Ir complexes, which were subsequently reacted with various metal precursors to afford a series of bimetallic complexes.

Particularly, in reactions with metal precursors, in addition to obtaining the expected structures coordinated through the second lone pair of the carbene (7-IrAu and 7-PdAu), we were surprised to discover that the Ir - CDC complex can oxidize the metal (9-Ir), while the CDC-Pd complex exhibits an additional reactive site on the imidazole ring, allowing for either coordination (8-PdAu) or carbon-carbon homocoupling reactions (9-Pd₂ and 10-Pd₂). Moreover, during the coupling reactions on the imidazole ring of 9-Pd₂ and 10-Pd₂, we detected EPR signals, indicating the formation of radical intermediates in the reaction process, which confirms that both mechanisms involve a radical pathway.

Keywords: Carbodicarbene, Bimetallic complex, Palladium complex, Iridium complex



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ISOLABLE TWO-COORDINATE GERMANIUM(II) DI-CATION

Yin-Zhi Weng,^{a,b} Lei Qin,^c Bamlaku Semagne Aweke,^b Lili Zhao,^c Glenn P. A. Yap^d
and Tiow-Gan Ong^{a,b *}

^a Department of Chemistry, National Taiwan University, Taipei, Taiwan (R.O.C)

^b Institute of Chemistry, Academia Sinica, Taipei, Taiwan (R.O.C)

^c School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing, China (P.R.C)

^d The Department of Chemistry and Biochemistry, University of Delaware, Newark, DE (USA)

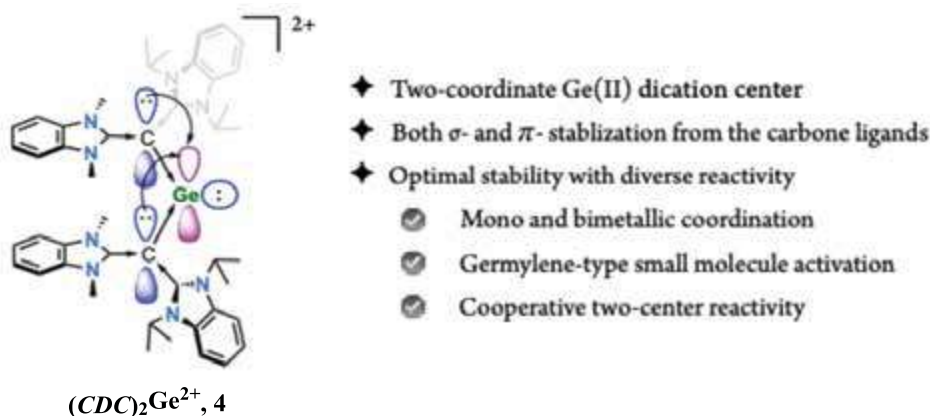
*Corresponding author: tgong@gate.sinica.edu.tw

Abstract

The germanium(II) dication species have been flourished in the decades. However, most of the reported works lacked reactivity at the Ge(II) center due to the involvement of multiple ligands or a high coordination number. Herein, we introduce only two neutral ligands, carbodicarbenes (CDCs), which are species that possess two lone pairs of electrons on their carbon atoms to stabilize the highly cationic Ge(II) atom, (CDC)₂Ge²⁺ (**4**). In this work, we characterized complex **4** by single-crystal X-ray diffraction (sc-XRD) and nuclear magnetic resonance (NMR) spectroscopy. DFT calculations reveal that the Ge(II) dication is stabilized not only by σ -donation but also by weak π -donation. Natural population analysis (NPA) assigns a charge of +0.77 to the Ge(II) center, indicating that the positive charge is shared by the carbodicarbene substituents. To investigate the reactivity of complex **4**, we successfully synthesized Rh(I) and Ir(I) complexes, demonstrating its capability as a cationic ligand. The bi-Ag(I) complex was facilely synthesized by treating **4** with two equivalents of AgOTf, which featured a unique 2-center-3-electron bonding mode. The Germylene-type ambiphilic nature was confirmed via small molecule activation, in which **4** underwent oxidative addition at the Ge(II) center.

Keywords:

Ge(II) di-cation, carbodicarbenes, cationic ligand



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AEROBIC PHOTODECOMPOSITION OF PYRENE-BASED METAL-ORGANIC FRAMEWORK NU-1000

Wenyi Zeng^{a,b}, Tristan T. Y. Tan^{a,*}, Jia Min Chin^{c,*}, Jason Y. C. Lim^{a,d,*}

^a*Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR), 2 Fusionopolis Way, Innovis #08-03, Singapore 138634, Republic of Singapore*

^b*Institute of Inorganic Chemistry, Faculty of Chemistry, University of Vienna, Währinger Str. 42, 1090 Vienna, Austria.*

^c*Institute of Functional Materials and Catalysis, Faculty of Chemistry, University of Vienna, Währinger Str. 42, 1090 Vienna, Austria.*

^d*Department of Materials Science and Engineering, National University of Singapore (NUS), 9 Engineering Drive, Singapore 117576, Republic of Singapore*

*Corresponding author: tristan_tan@imre.a-star.edu.sg, jiamin.chin@univie.ac.at, jason_lim@imre.a-star.edu.sg

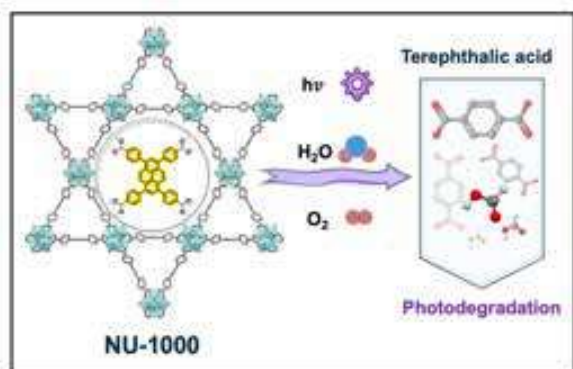
Abstract

NU-1000, a widely studied pyrene-based metal-organic framework (MOF), is valued for its structural robustness and versatility in various photochemical applications. While its extended π -conjugation enhances light-absorbing properties, it also renders the framework more vulnerable to photodegradation. Despite its extensive use, the photostability of NU-1000 has not been systematically investigated. In this work, we demonstrate that NU-1000 undergoes significant photodecomposition in the presence of O₂, water and UV radiation, primarily yielding terephthalic acid as the major degradation product. The product was characterized by NMR, high-resolution ESI-MS. Through mechanistic studies, we reveal that the porous architecture of NU-1000 substantially accelerates linker oxidation, resulting in over 25-fold higher degradation of the linker compared to the free ligand in solution after 3 hours of irradiation. This enhancement is attributed to the efficient in situ generation of carbon centered holes localized on the ligand within the framework.

Our findings not only establish a clearer understanding of the photo-instability of NU-1000 but also define the specific conditions required to maintain its structural integrity. Furthermore, the ability of NU-1000 to degrade into environmentally benign products under ambient conditions presents a promising strategy for minimizing the persistence of MOF materials in the environment. This study offers valuable insights for both extending the practical utility of NU-1000 and guiding the design of more sustainable MOF systems.

Keywords: Metal-organic frameworks, NU-1000, photodegradation

Graphic / Image



HYDROGENOLYSIS OF XYLITOL TO ALCOHOLS AND DIOLS OVER NICKEL SUPPORTED ON MIXED METAL OXIDES

Mzamo L Shoji^{a,*}, Vuyolwethu Ndabankulu^a, Alisa Govender^b, Holger B. Friedrich^a

^a*School of Chemistry and Physics, University of KwaZulu-Natal, Westville Campus, Durban, 4000, South Africa.*

^b*Department of Chemistry, Durban University of Technology, P.O Box 1334, Durban 4000, South Africa.*

**Corresponding author: shozim2@ukzn.ac.za*

Abstract

Hydrogenolysis of xylitol produces value-added diols such as ethylene glycol (EG), 1,2-propanediol (1,2-PDO), and alcohols such as methanol, ethanol and propanols. EG and 1,2-PDO are used in many industrial processes as raw materials in heat-transfer fluid industries, as monomers in the manufacture of polyester resins, and in pharmaceutical, cosmetics, and packaging industries [1, 2]. Generally, the hydrogenolysis of xylitol requires the use of supported metal catalysts (i.e Pt, Ru, Ni, Cu) and the addition of a homogeneous base. Nickel catalysts have been shown to have high activity in the hydrogenolysis reactions under hydrogen pressure and elevated temperatures [3]. Mixed metal oxide alumina supports were prepared by the co-precipitation method and impregnated with nickel to form the supported catalysts. Powder x-ray diffraction (XRD) was used to determine the phases in the material. Temperature programmed reduction (TPR) was used to understand catalyst reducibility. CO₂-Temperature programmed desorption (TPD) was used to quantify the basic sites of the support and catalysts. Xylitol hydrogenolysis reactions were carried out in a high-pressure stainless-steel autoclave. N₂ physisorption data showed that all the prepared materials were mesoporous and had a high BET surface area. In all the prepared catalysts Ni was reducible at temperatures below 500 °C, which meant that the risk of sintering was minimized. Incorporating the base in the alumina structure improved the catalytic activity and selectivity towards diols and alcohol under mild reaction conditions.

Keywords: nickel catalysts, hydrogenolysis, xylitol, diols, alcohols

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HIDDEN FRUSTRATED LEWIS PAIRS BASED ON CARBODICARBENE - BORANE COMPLEXES

Po-Hung Huang^{a,b}, Geetanjali S. Sontakke^a, Jiun-Shian Shen^{a,b}, Yin-Zhi Weng^{a,b}, Bamlaku Semagne Aweke^a, Glenn P. A. Yap^c, and Tiow-Gan Ong^{*a,b}

^a Institute of Chemistry, Academia Sinica, Taipei (Taiwan, ROC)

^b Department of Chemistry, National Taiwan University, Taipei (Taiwan, ROC)

^c Department of Chemistry and Biochemistry, University of Delaware, Newark, DE (USA) *

*Corresponding author: tgong@gate.sinica.edu.tw

Abstract

In this study, carbodicarbenes (CDCs) were integrated into frustrated Lewis pair (FLP) chemistry by pairing them with boron-based Lewis acids, specifically $B(C_6F_5)_3$ and BPh_3 , leading to the synthesis and full characterization of novel CDC-boron complexes. Among them, complex **2a** (C_1 -CDC- BPh_3) exhibited unexpected FLP-like reactivity despite forming a stable Lewis adduct, activating small molecules such as benzyl alcohol, diphenylamine, and phenylacetylene through O-H, N-H, and C-H bond cleavage to generate ion-pair products. It also successfully mediated hydride abstraction from pinacol borane and phenyl silane and activated carbon dioxide to form a CO_2 -bridged zwitterionic adduct. Mechanistic studies, supported by DFT calculations, highlighted the crucial role of the combination of CDC and BPh_3 in enhancing reactivity. Building on this, the catalytic potential of CDC-boron complexes was explored, with **2a** catalyzing the hydroboration of various ketones under mild conditions with high efficiency and functional group tolerance. Additionally, hydrosilylation of ketones was achieved using the ' Pr_4 -CDC/ BPh_3 ' pair as a catalyst. Overall, this work demonstrates the versatility of CDC-based FLPs in small molecule activation and catalytic applications.

Keywords: Carbodicarbene, Frustrated Lewis Pair, hydroboration, hydrosilylation

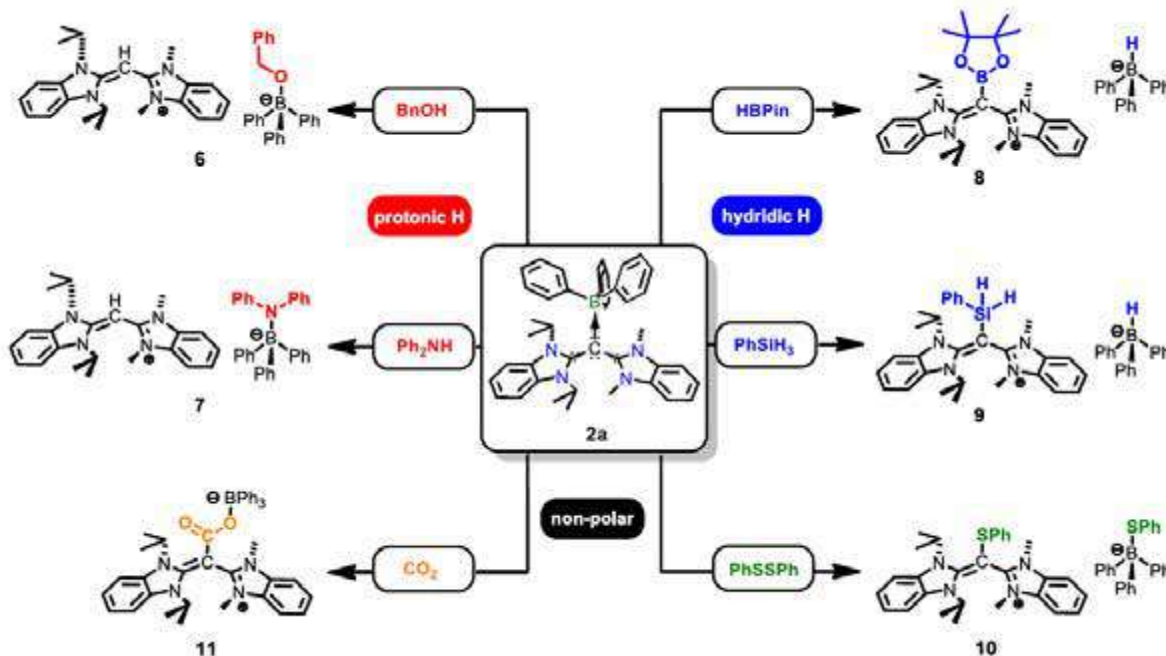


Figure 1 The diversity of **2a** reacts with small molecules

QUANTITATIVE STUDY ON THE INFLUENCE OF BROMIDE IONS TOWARD THE REDUCTION KINETICS FOR SIZE-TUNABLE PALLADIUM NANOCUBES

Yilin Zhao^a, Jianzhou Wu^{a,*}, Jie Fan^{a,*}

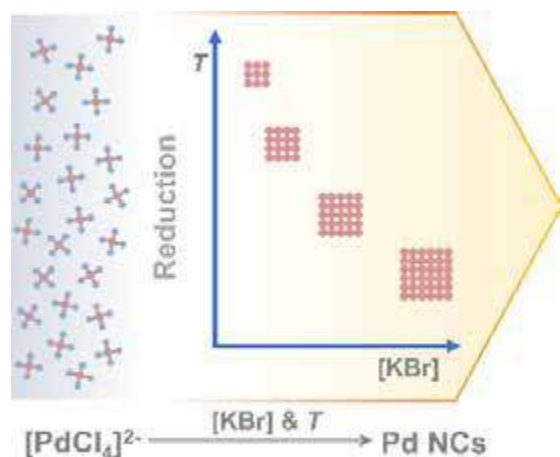
^aKey Lab of Applied Chemistry of Zhejiang Province, Department of Chemistry, Zhejiang University, Hangzhou 310058, China

*Corresponding author: jfan@zju.edu.cn

Abstract

During the preparation of nanocrystals, regulating the dosage of key additives in the reaction system and the reaction temperature commonly affect the sizes and morphologies of the products. It is generally accepted that the concentration of bromide ions in reaction system can impact the reduction kinetics of Pd precursor, further controlling the outcome of Pd nanocubes (Pd NCs). However, nearly two decades since the first time this perspective was proposed, there is still a lack of quantitative understanding or description of their kinetic characteristics under different reaction conditions. In this work, Pd NCs with different sizes have been prepared under various reaction conditions coupled with a systematic mechanism study. Quantitative measurements demonstrate that the reduction processes could be considered as quasi-first-order reactions, and the corresponding kinetic parameters have been obtained. Furthermore, a linear relationship is discovered between k and the average size (d) of Pd NCs. The investigation on the growth patterns of four chosen systems reveals that given reaction conditions lead to certain results with unique growth patterns. This work provides detailed illustrations on the preparation of size-tunable Pd NCs, and offers a systematic view toward the growth pattern.

Keywords: Palladium cubic nanocrystal, additive, reaction temperature, reduction rate constant, growth pattern



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PERFORMANCE ANALYSIS OF GLDA AND HEDTA AS CHELATORS FOR CALCIUM AND FERRUM IONS AT 80 °C

^{a, b}Ahmad Shalabi Md Sauri, ^cKarimah Kassim, ^aEmily S Majanun, ^cMohd Fazli Mohamat, ^dNajmiddin Yaakob, ^cMuhamad Kamil Yaakob, ^aAhmad Zahir Hafiz, ^aFarhana Jaafar Azuddin.

^aPETRONAS Research, 43000 Kajang Selangor, Malaysia.

^bFaculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia.

^cInstitute of Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia.

^dFaculty of Chemical Engineering, 40450 Shah Alam, Selangor, Malaysia.

*Corresponding author: karimah@uitm.edu.my

Abstract

Chelators are chemical compounds that bind to metal ions, forming stable complexes and preventing these ions from participating in undesirable chemical reactions. Their ability to control metal ion availability and prevent scale formation makes them valuable across numerous industries, including industrial cleaning, medicine, agriculture, water treatment, oil and gas, cosmetics, and the food industry. In the oil and gas sector, particularly effective chelators are essential as additives in production chemicals, especially those that remain stable under highly acidic conditions (pH 1–3). However, the availability of chelators that can effectively function under such harsh conditions is limited. This study aims to evaluate the performance of tetrasodium glutamate diacetate (GLDA) and hydroxyethylenediamine triacetic acid (HEDTA) as chelators for calcium (Ca²⁺) and iron (Fe²⁺) ions in these extreme conditions across various temperatures. The performance of these chelators was assessed through computational methods, including Density Functional Theory (DFT) and Monte Carlo simulations. DFT quantum chemistry calculations indicated that GLDA potentially offers superior electron transfer capabilities, resulting in stronger adsorption properties compared to HEDTA. Additionally, Monte Carlo calculations revealed that GLDA exhibits slightly higher adsorption energy than HEDTA. Experimental results further supported these findings. For calcium ions (Ca²⁺) at pH 3, GLDA proved to be a more effective chelator than HEDTA, while HEDTA performed better at pH 1. Regarding iron ions (Fe²⁺), GLDA outperformed HEDTA at both pH levels, demonstrating its superior chelating ability. These insights suggest that GLDA may be a more robust and versatile chelator for use in the highly acidic environments typical of oil and gas production, providing a potential solution to the current limitations in effective chelation under such conditions.

Keywords: chelators, oil and gas, HEDTA, GLDA, molecular modeling

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DEVELOPING NEW SYNTHETIC METHODOLOGIES OF DEAROMATIZATION REACTIONS

Shu-Li You*

*New Cornerstone Science Laboratory, State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences
345 Lingling Lu, Shanghai 200032, China*

**Corresponding author: slyou@sioc.ac.cn*

Abstract

Dearomatization reactions are widely recognized as powerful methods for the synthesis of highly functionalized three-dimensional structures from simple planar aromatic compounds. Among those, catalytic asymmetric dearomatization (CADA) reactions are very attractive due to the abundance and ready availability of aromatic compounds and the direct access to enantiopure polycycles and spirocycles offered by them. That latter are frequently the key motifs in biologically active natural products and pharmaceuticals. However, due to the extra stability of “aromaticity” of the arenes, their dearomatization reactions with good enantioselective control has been a great challenge. In this talk, we present our recent results toward the development of new dearomatization reactions. The dearomatization reactions of indoles, pyrroles, phenols, naphthols, and pyridines have been achieved, affording various highly functionalized heterocycles bearing all-carbon quaternary chiral centers in most of the cases. These results provide not only the efficient synthesis of highly enantioenriched spiro- or polycycles, but also a novel concept in synthetic methodology development.

Keywords: Insert maximum of 5 keywords

Aromatic compounds; asymmetric catalysis; dearomatization; homogenous catalysis; synthetic reaction

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CHIRAL SPIRO CATALYSTS FOR ASYMMETRIC HYDROGENATION OF KETONES

Qi-Lin Zhou

College of Chemistry, Nankai University

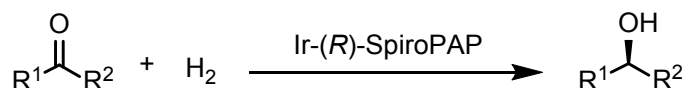
Tianjin 300071, China

Email: qlzhou@nankai.edu.cn

Abstract

Chiral catalysts are the key for the catalytic asymmetric synthesis. In last few decades, many chiral catalysts have been developed. However, most of the reported chiral catalysts showed high activity and high enantioselectivity for limited reactions, sometime for only limited substrates. Very few chiral catalysts provided satisfying activity and enantioselectivity for a wide range of mechanistically unrelated reactions. In the last two decades, we have developed a new type of chiral catalysts with a spirobiindane framework. Chiral spiro catalysts exhibited excellent activity and enantioselectivity for wide range of reactions, such as asymmetric hydrogenation, carbon-carbon bond and carbon-heteroatom bond-forming reactions. This lecture will present the design and synthesis of chiral spiro catalysts and their applications in the asymmetric hydrogenation of ketones.

Keywords: Chiral catalyst; Spiro ligand; Ketone; Asymmetric hydrogenation.



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RECONSTRUCTING BIOSYNTHETIC PATHWAYS FOR COMPLEX FUNGAL NATURAL PRODUCTS

Emily J Parker^{a,*}

^a*Ferrier Research Institute, Victoria University of Wellington 6140, New Zealand.*

^{*}*Corresponding author: emily.parker@vuw.ac.nz*

Abstract

Many organisms, including plants and microbes, utilise unique armouries of bioactive compounds provide protection against predators and enable establishment of new ecological niches. Although bioactive compounds are used widely for industrial and pharmaceutical applications their diversity remains largely untapped as many compounds are produced in very low yields and the complexity of their biosynthesis is yet to be fully understood.

The indole diterpenes (IDTs) class of fungal natural products that have attracted widespread interest due to their remarkable chemical diversity and attendant bioactivities, which include anti-bacterial, anti-viral, anti-cancer and insecticidal properties. By using heterologous expression and employing our new molecular biology tools, we have reconstructed biosynthetic pathway of some unusual and potentially valuable IDTs in an alternative fungal host. Our work has uncovered large natural product compound arrays, allowing access to many known and novel compounds.

Keywords: Indole diterpenes, filamentous fungi, heterologous biosynthesis

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P-CHIROGENIC ORGANOPHOSPHORUS COMPOUNDS: AXIS TO CENTER CHIRALITY TRANSFER REACTION

Toshiaki Murai*

Department of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University, Yanagido,
Gifu 501-1193, Japan

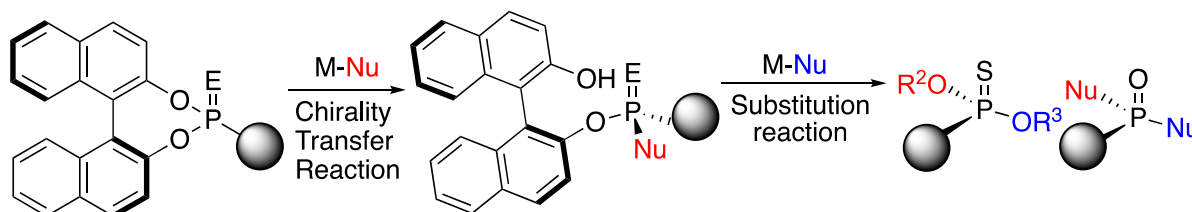
Corresponding author: murai.toshiaki.u6@a.gifu-u.ac.jp

Abstract

P-Chirogenic organophosphorus compounds play a crucial role due to their extensive applicability as drugs, prodrugs, optically active ligands, and organocatalysts. Over the past three decades, a variety of synthetic methods have been developed, including kinetic resolutions, desymmetrization of prochiral organophosphorus compounds, and the separation of diastereomixtures. In this context, we have developed axis-to-central chirality transfer reactions involving pentavalent four-coordinate organophosphorus compounds bearing a binaphthyl group.¹ We have also explored the conversion of the resulting compounds into enantiomerically enriched P-chirogenic organophosphorus compounds. As key starting materials, we devised organophosphoroselenoyl chlorides by reacting PCl_3 , elemental selenium, and optically active bi-2-naphthols. The resulting chlorides reacted with oxygen-, nitrogen, and carbon-containing nucleophiles. The selective substitution reaction at the phosphorus atom proceeded with high efficiency to give the compounds with P-O, P-N and P-C bonds. The replacement of a P=Se bond with a P=O bond was readily achieved by reacting with hydrogen peroxide. As an illustrative example of the further reaction, the sequential substitution reaction of phosphonates with a binaphthyl group using aromatic Grignard reagents and methyl Grignard reagents proceeded smoothly, yielding enantiomerically enriched P-chirogenic phosphine oxides in high yields with high enantiomeric ratios.² These two-step reactions entail the transfer of axial chirality from the binaphthyl group to the central chirality of the phosphorus atom, coupled with a stereoselective substitution reaction of the initial products with Grignard reagents. Key substrates employed in these reactions included phosphinates,³ phosphates,⁴ phosphorothioates,⁴ and phosphonothioates⁵ with a binaphthyl group, which reacted with hydroxides and alkoxides as nucleophiles. Further details regarding these reactions will be provided.

Keywords: P-chirogenic; organophosphorus compounds; axial chirality; central chirality; chirality transfer

Graphic / Image (Optional)



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BORON CAGE EXTENSION STRATEGY WITH AROMATIC HETEROCYCLES

Jordi Poater^{a*}, Deshuang Tu^b, Miquel Solà^c, Hong Yan^b

^aICREA and Universitat de Barcelona, Barcelona, Spain.

^bNanjing University, Nanjing, China.

^cUniversitat de Girona, Girona, Spain.

*Corresponding author: jordi.poater@ub.edu

Abstract

Heteropolycyclic molecular systems, which are essential components in the fields of materials science and pharmacology, are often composed of 2D extended aromatic rings. Here, we introduce a class of 3D aromatic boron cluster-fused heterocyclic phosphoniums by merging a nido-carborane cage with a phosphine and a π -conjugated unit.¹ To achieve this, we developed a new synthetic methodology that encompasses Pd(II)-catalyzed,^{2,3} P(III)-directed B–H activation of nido-carboranes with alkynes. This method facilitates the production of a diverse array of carborane-extended phosphoniums with high yields under mild conditions. The inclusion of the carborane moiety leads to a twisted molecular structure, resulting in increased stability compared to their 2D planar counterparts. Moreover, the fusion between the 3D boron cluster^{4,5} and the novel five-membered borophosphonium heterocycle enables electron delocalization across the structure. This unique feature transforms the inherent photo-inert properties of the carborane cage into high-performance luminogens with a range of emission behaviors, including aggregation-induced emission (AIE), highly efficient tunable color solid-state luminescence, and aggregation-induced circularly polarized luminescence. Consequently, this groundbreaking boron cluster-fused phosphonium framework significantly expands the library of aromatic-based heterocycles and demonstrates considerable promise for applications in functional materials.

Keywords: heterocycle; aromaticity; DFT; boron cage.



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DEVELOPMENT OF ARTIFICIAL WATER CHANNELS THROUGH SMALL-MOLECULE SELF-ASSEMBLY

Pinaki Talukdar^{a,*}

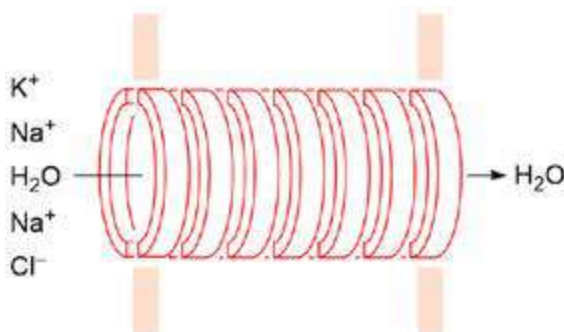
^aDepartment of Chemistry, Indian Institute of Science Education and Research Pune, Dr. Homi Bhabha Road, Pashan, Pune 411008, India

*Corresponding author: ptalukdar@iiserpune.ac.in

Abstract

Aquaporins are specialized protein channels embedded in biological membranes that enable the rapid and highly selective transport of water molecules. Their exceptional permeability (each channel can transport approximately 10^9 water molecules per second) and remarkable selectivity, allowing only water to pass while fully rejecting solutes, have drawn significant interest. In reverse osmosis (RO) membranes, incorporating aquaporins can enhance both permeability and selectivity, leading to reduced energy consumption compared to conventional RO systems. Researchers are actively exploring bio-inspired membranes with embedded aquaporins to advance desalination and water purification technologies. However, as protein molecules, aquaporins present challenges related to stability under harsh conditions and scalability. To overcome these limitations, scientists are developing synthetic analogs that replicate the efficiency and selectivity of aquaporins. By mimicking their structural and functional properties, researchers aim to create advanced artificial membranes for applications in water purification and desalination. In this seminar, we will discuss recent strategies for designing artificial water channels, covering their design, synthesis, and water transport properties. Their ability to selectively discriminate species such as cations, anions, and protons will also be highlighted. Additionally, insights into their water transport mechanisms, derived from theoretical studies, will be presented.

Keywords: Aquaporin, Reverse osmosis, Artificial water channel, Light scattering, Fluorescence



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ASYMMETRIC CATALYSIS WITH CARBOCATION SURROGATES

Craig P. Johnston^{a,*}

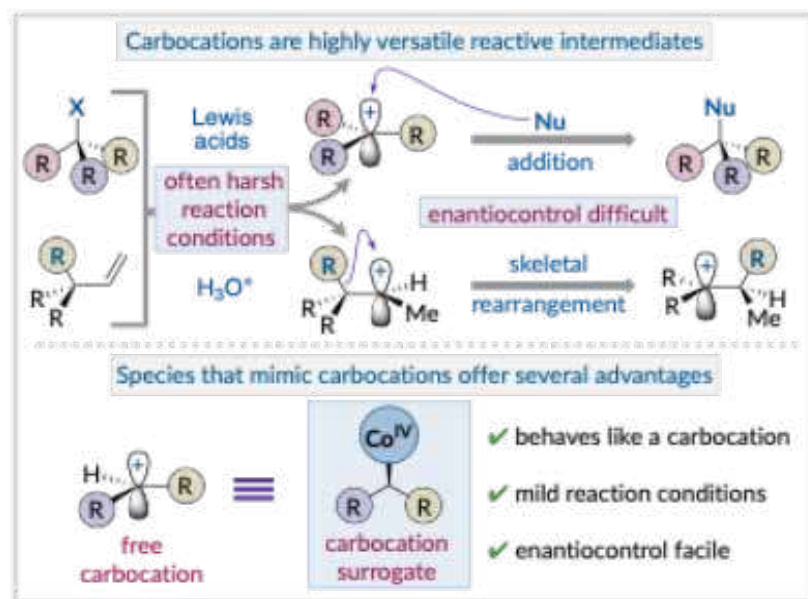
^a*EaStCHEM, School of Chemistry, University of St Andrews, UK*

**Corresponding author: cpj3@st-andrews.ac.uk*

Abstract

Carbocations are synthetically useful reactive intermediates as they can enable distinct transformations, such as nucleophilic additions and the structural reorganisation of the molecule's framework. However, their generation often requires harsh reagents (e.g. strong acids) and struggles with the formation of unstabilised carbocations. Equally, the low energetic barriers associated with carbocation reactivity pose significant challenges for achieving stereocontrol. Therefore, these factors have historically constrained the use of carbocations in stereoselective synthesis. Our objective was to develop a strategy to access carbocation-type reactivity under milder, more selective conditions using cobalt-based surrogates. We hypothesised that alkylcobalt(IV) intermediates could serve as functional stereodefined mimics of carbocations in key bond-forming reactions. These intermediates were then shown to facilitate transformations, such as 1,2-aryl migrations^{1,2} and olefin hydration.³ The conditions for these reactions are generally mild and non-acidic offering improved chemoselectivity and functional group tolerance. Furthermore, these transformations can be rendered enantioselective using a chiral salen ligand coordinated with the cobalt catalyst.

Keywords: Cobalt, HAT, carbocation, enantioselective, homogeneous catalysis



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INTRAMOLECULAR VS INTERMOLECULAR ZWITTERIONIC ACYLPYRAZOLONE LIGANDS AND THEIR SPONTANEOUS COORDINATION WITH CESIUM CARBONATE

Vanya B. Kurteva^{a,*}, Stanislava E. Todorova^a, Rusi I. Rusew^b, Boris L. Shivachev^b

^a*Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 9, Sofia 1113, Bulgaria*

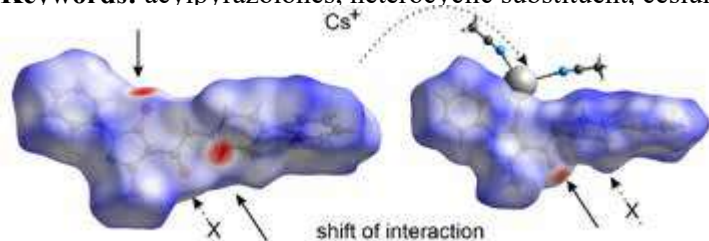
^b*Institute of Mineralogy and Crystallography "Acad. Ivan Kostov", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 107, Sofia 1113, Bulgaria*

*Corresponding author: vanya.kurteva@orgchm.bas.bg

Abstract

Acylpyrazolones are among the most widely used chelating extractants due to their excellent coordination properties.^{1,2} Herein, we present the synthesis and characterization of a series of acylpyrazolones possessing a methylene bridged heterocyclic unit in the acyl fragment, i.e. combining the structural units of the extractant and the synergist of the extraction process in a common molecule. It is found that the products exist in the solid state as intramolecular or intermolecular zwitterions between the tautomeric pyrazolone hydroxyl group and the nitrogen atom of the acyl substituents. The single crystal XRD data revealed that the ligands possessing 6–8-membered heterocyclic units crystallize as an intramolecular zwitterion with the heterocyclic fragment oriented towards enolate (group 1), those containing 5-membered pyrrolidine and *N*-phenylpiperazine as an intermolecular zwitterion with the heterocyclic fragment oriented opposite to enolate (group 2), while the 1-aza-12-crown-4 derivative as an intramolecular zwitterion with the heterocyclic fragment oriented opposite to enolate (group 3). It is ascertained that the products coordinate spontaneously with cesium carbonate used as the base and that the complexes formed are not stable on silica gel and decompose during chromatography to free ligands. It is shown that the coordination pattern is closely related with the free ligand orientation; the ligands of group 1 coordinate with cesium with the two oxygen atoms of the pyrazolone unit, those of group 2 only with the oxygen atom of the tautomeric hydroxyl group, and that of group 3 with aza-crown ether heteroatoms. It is found that the starting chloride also coordinates to cesium carbonate and it is proved that this complex does not participate as a reaction intermediate, i.e. the ligands are initially formed followed by coordination with cesium carbonate.

Keywords: acylpyrazolones, heterocyclic substituent, cesium complexes, NMR, single crystal XRD



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A SINGLE BIOORTHOGONAL REACTION FOR MULTIPLEX CELL SURFACE PROTEIN LABELING

Yu-Hsuan Tsai

Institute of Molecular Physiology, Shenzhen Bay Laboratory; Shenzhen, China.

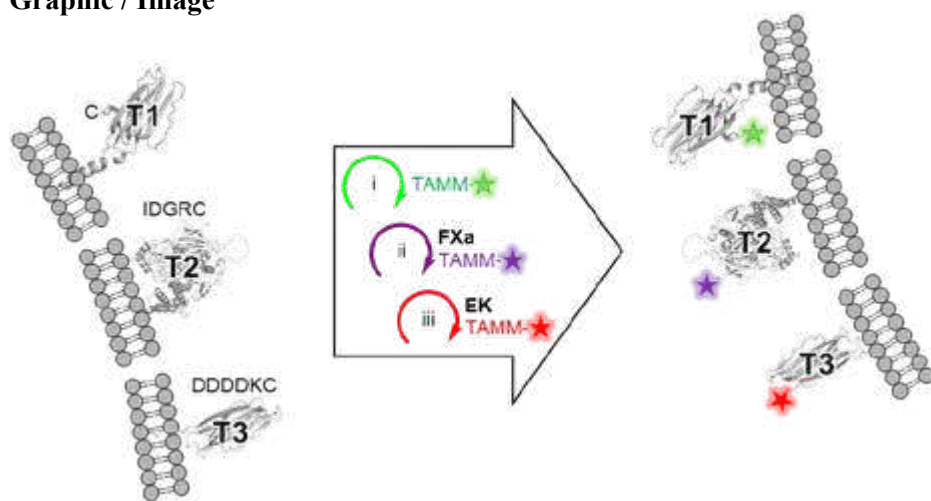
**Corresponding author: tsai@szbl.ac.cn*

Abstract

Small-molecule fluorophores are invaluable tools for fluorescence imaging. However, means for their covalent conjugation to the target proteins limits applications in multi-color imaging. Here, we identify 2-[(alkylthio)(aryl)methylene]malononitrile (TAMM) molecules reacting with 1,2-aminothiol at rate constant up to $10^4 \text{ M}^{-1} \text{ s}^{-1}$ through detailed mechanistic investigation. The ultrafast TAMM molecules and mild reaction conditions enable specific labeling of surface proteins in not only cell lines but also primary neurons and living mice. Combination of genetic code expansion and sequence-specific proteolytic cleavage enables selective modification of three different cell surface proteins through iterative TAMM condensation. TAMM condensation is also compatible with Cu-catalyzed azide–alkyne cycloaddition and tetrazine ligation for four-color fluorescent labeling, reaching the maximum available colors of conventional confocal microscopes. Thus, bioconjugation chemistry is no longer the limiting factor for live-cell multiplex surface protein imaging.

Keywords: 1,2-aminothiol, bioorthogonal chemistry, site-specific protein modification, fluorescent labeling, genetic code expansion

Graphic / Image



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APPLICATION OF PHOTOPHARMACOLOGY IN AGROCHEMICALS

Xusheng Shao^{a,,b,c,*}

^aShanghai Key Laboratory of Chemical Biology, School of Pharmacy, East China University of Science and Technology, Shanghai, 200237, China; ^bState Key Laboratory of Bioreactor Engineering, East China University of Science and Technology, Shanghai 200237, China; ^cShanghai Frontier Science Research Base of Optogenetic Techniques for Cell Metabolism, School of Pharmacy, East China University of Science and Technology, Shanghai 200237, China

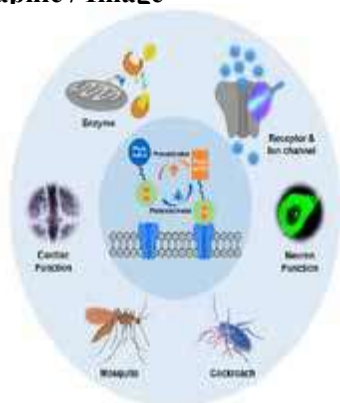
*Corresponding author: shaoxusheng@ecust.edu.cn

Abstract

Photopharmacology is a novel technology in drug design that aims at solving poor drug selectivity. This technology, currently in the proof-of-concept phase, relies on the photoactivation or inactivation of photochromic ligands (PCLs) to regulate biological functions and living organisms. As potential molecular tools in future agriculture 4.0, the photochromic pesticides are effective in optical control of receptors, ion channels, living behaviors, and enzymes, displaying an innovative way of pesticide discovery. By integrating photoswitches, such as azobenzenes and diarylethenes, into pesticide molecules, we obtained several PCLs for optical regulations of GABARs, RyRs, nAChRs, SURs, sodium channels, GluClRs, and SDH that are important targets in vivo of insects or fungi. The results are indeed meaningful in elucidating interactions of agrochemicals on targets, biological functions, and living behaviors, providing powerful toolkits in understanding ligand-receptor interactions. We envision that this particular mode of pesticide discovery is promising in the circumvention of undesired problems that are caused by the improper use of agrochemicals.

Keywords: photopharmacology, light, agrochemicals, insect, fungi

Graphic / Image



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IDENTIFICATION OF FURANYL- AND THIOPHENYL-3-PHENYL-1*H*-INDOLE-2-CARBOHYDRAZIDE DERIVATIVES AS POTENT ANTI-TUBULIN AND ANTICANCER AGENTS

Chatchakorn Eurtivong^{a,*}, Rungroj Saruengkhanphasit^b

^aMahidol University.

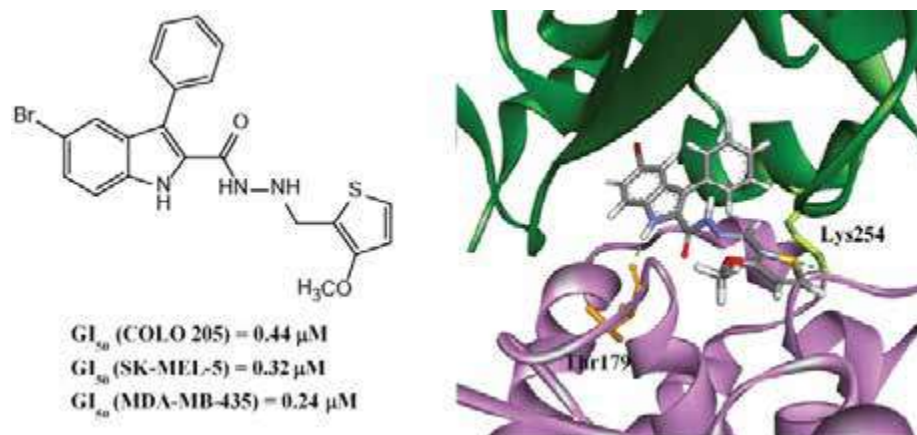
^bChulabhorn Graduate Institute

*Corresponding author: chatchakorn.eur@mahidol.edu

Abstract

Tubulin has been established as a successful drug target. Over the years, the *Vinca* alkaloid drug class, which includes paclitaxel, docetaxel, vinblastine and vincristine has been the epitome of anti-tubulin drugs for the treatment of various cancer types. Regardless, emergence of drug resistance and side effects are major drawbacks, and intravenous injection has been the only way of drug administration for this drug class leading to patient compliancy issues. Thus, orally available anti-tubulin agents are suggested as improved alternatives. Despite this, none have yet made it successfully to the clinic. In our project, the furanyl- and thiophenyl-3-phenyl-1*H*-indole-2-carbohydrazides were identified from a virtual high throughput screening campaign as new series of anti-tubulin agents with potent anticancer activities. The structure-activity relationships (SARs) of both the thiophenyl and furanyl series were developed through synthesis and biological evaluation. Herein we will discuss the initial virtual screening methods,¹ SAR development,^{1,2} and the clinical potential of the series.² Based on the results, the series were most selective and effective at inhibiting the growth of colon, melanoma and breast cancers with GI₅₀ and LC₅₀ values in the submicromolar range, *i.e.*, <1 mM.² The pharmacokinetic profiles of the derivatives were predicted *in silico* to be compatible for oral drug administration.

Keywords: tubulin, anticancer drugs, virtual screening, synthesis, pharmacokinetics



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GOLD-CATALYZED AND NaH-SUPPORTED CYCLIZATION OF N-PROPARGYLATED PYRROLE AND INDOLE: SYNTHESIS OF HETEROCYCLES WITH NEW SCAFFOLDS

Metin Balci

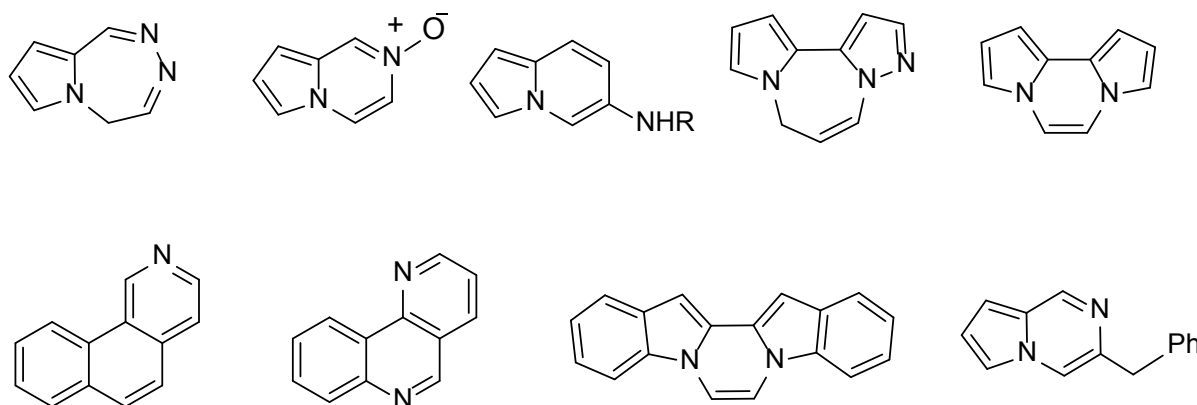
Department of Chemistry, Middle East Technical University, 06800 Ankara, Turkey

*Corresponding author: mbalci@metu.edu.tr

Abstract

Compounds classified as heterocyclic probably constitute the largest and most varied family of organic compounds and they are well presented among pharmaceuticals. As part of our ongoing research program on the design and synthesis of heterocycles with new skeletons we developed new methodologies. The key feature of this methodology was the synthesis of N-propargyl pyrrole, indole, and benzene derivatives. Gold-catalyzed or NaH-supported cyclization of these compounds resulted in the formation of compounds given below[1-10]. The gold-catalyzed reaction of pyrrole and indole oximes having N-propargyl group transferred the oxime functionality intramolecularly from one carbon atom to another carbon atom via 7-endo-dig cyclization process. This transformation is unprecedented in the literature and was named as oxime-oxime rearrangement.[4]

Keywords: Alkyne cyclization, pyrrole, indole, oxime-oxime rearrangement, propargyl rearrangement



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ENANTIOSELECTIVE C–P AND C–C BOND FORMATION THROUGH C(sp³)–H FUNCTIONALIZATION

Sandra Ardevines^a, Christian Ascaso-Alegre^a, M. Concepción Gimeno^a, Juan Mangas-Sánchez^b,
Eugenia Marqués-López^a, Raquel P. Herrera^{a,*}

^a*Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), CSIC- University of Zaragoza.
E-50009 Zaragoza, Spain*

^b*IUQOEM, School of Chemistry, University of Oviedo. Julián Clavería 8, 33006 Oviedo, Spain
Corresponding author: raquelph@unizar.es*

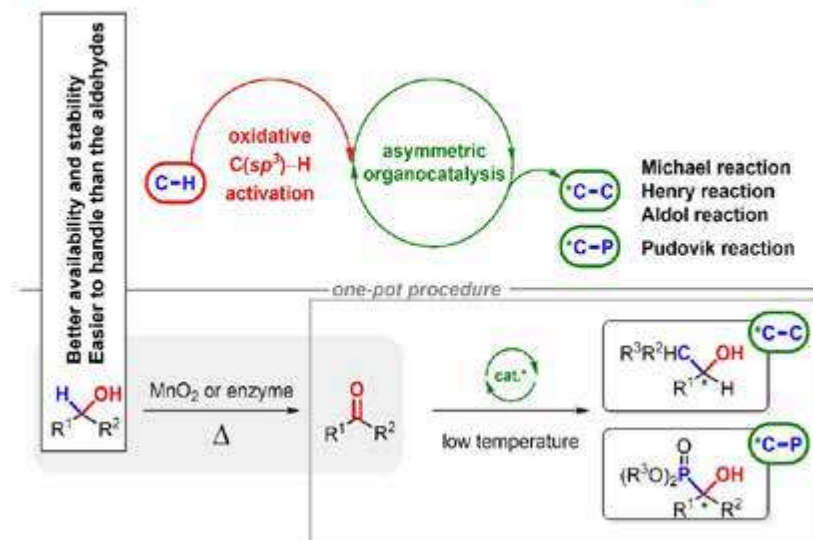
Abstract

Many organic reactions involving aldehydes lead to products of biological interest. However, aldehydes are easily contaminated over time by traces of their corresponding carboxylic acids, which can inactivate organocatalysts, as observed during our previous Henry protocol development.^[1] Motivated by this observation, we explored the possibility of producing aldehydes *in situ* by oxidizing the corresponding alcohols.^[2] Alcohols are more convenient than aldehydes, mainly due to their higher availability, stability, and ease of handling. The transformation of alcohols into the corresponding carbonyl compounds for subsequent reaction with nucleophiles in an organocatalytic and enantioselective manner has been scarcely investigated.

Herein, we present the pioneering work and the first organocatalytic enantioselective aldol,^[2] Henry,^[2,3] Pudovik^[3,4] and Michael^[4] reactions starting from alcohols through a formal C(sp³)-H activation, important methods for forming C-C and C-P bonds in organic synthesis.

Keywords: cascade, enzymes, one-pot, organocatalysis, oxydation

Organocatalyzed Aldol, Henry, Pudovik and Michael Reaction starting from Alcohols



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AMINOPIPERIDINES AND DERIVATIVES AS ANTI-PAF/ANTI-HIV-1 ANTAGONISTS. SYNTHESIS AND MOLECULAR MODELLING

Benmehdi Houcine^{a,*}, Lamouri Aazdine^b

^a *Laboratory of Chemistry and Environmental Sciences, Faculty of Technology, University of Bechar-Tahri Mohamed, BP 417. 08000. Bechar, Algeria.*

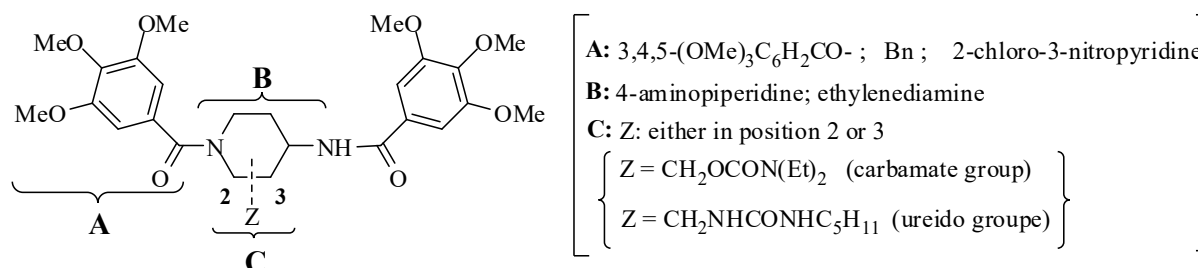
^b *Laboratoire ITODYS, Synthèses Organiques 15, rue de Baïf, 75205 Paris cedex 13 France*

* Corresponding author: h_ben90@yahoo.fr

Abstract

Excessive levels of PAF and cells of macrophage lineage appear to play an important role in neuronal cell injury, inflammatory syndrome, and HIV replication in CNS resulting in AIDS dementia complex. The beneficial effects of PAF receptor antagonists are evident and give rise to expected therapeutic strategies for neurotrauma. We therefore synthesized a novel class of 4-aminopiperidines and ethylenediamine substituted in the position 2 or 3 by groups bearing a carbamate or ureido function. Several substituents were introduced on one or both nitrogens of the 4-aminopiperidine and ethylenediamine rings in order to modify either lipophilicity, electronic distribution or steric effect. Their influence on both anti-PAF and anti-HIV-1 activities was also investigated. Our findings revealed that the most compounds were found to be able to diminish both HIV-1 replication in monocyte-derived macrophages and PAF induced platelet aggregation. Moreover, a molecular modelling analysis has been triggered to calculate 3D electrostatic potential maps of selected compounds and to study the conformational space of the nitrogen-containing derivatives.

Keywords: aminopiperidine, ethylenediamine, synthesis, PAF, HIV



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DUAL-AXIS ALIGNED THERMOPHILIC ARTIFICIAL WATER CHANNELS FORMED BY WATER-INDUCED SELF-ASSEMBLY

Chien-Lung Wang^{a,*}

^a Department of Chemistry, National Taiwan University, Taipei 10617, Taiwan.

*Corresponding author: kclwang@ntu.edu.tw

Abstract

Nature modulates the non-covalent interaction of biomolecules to strengthen their structural integrity against various extreme environments. Water, as the key component in living systems, provides the H-bonded connectivity to readily stabilize the thermophilic proteins toward thermal adaption. However, this strategy has seldom been utilized in synthetic matter since the role of water is less explored in the supramolecular chemistry of synthetic systems. In this study, we design a dendritic amphiphile that forms the hydrated hexagonal columnar (Col_h) phase in water-induced self-assembly (WISA).^{1,2} Characterization data show that the artificial water channels (AWCs) in the hydrated Col_h phase contain both the bulk-like and interfacial water in the hydrophilic core of the AWC.³ The H-bonded network of the embedded water molecules makes the AWCs thermophilic and prevents them from isotropization at temperatures even higher than the boiling point of water. Moreover, the weakened H-bonded network at high temperatures accelerates water flow through the dual-axis aligned AWCs and resulted in high water permeabilities. The study thus revealed the essential role of water in enhancing the thermophilic properties of the synthetic soft matter, which allows them to perform better functions at higher temperatures.

Keywords: self-assembly, supramolecular chemistry, artificial water channels, X-ray diffraction

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SYNTHESIS AND ISOMERIZATION OF AZOBENZENE-CYCLOPARAPHENYLENE MACROCYCLES FOR RESPONSIVE MATERIALS

Wei-Tzu Huang^{a*}, Masaki Horie^a

^aDepartment of Chemical Engineering, National Tsing Hua University, Taiwan (ROC).

*Corresponding author: vicky89106@gmail.com

Abstract

Cycloparaphenylenes (CPPs), known for their nonpolar π -orbital structures, have become increasingly attractive and significant in materials science, supramolecular chemistry, and physical sciences due to their distinctive electronic properties. Meanwhile, azobenzene, a well-known stimuli-responsive molecule, is recognized for its reversible *trans*-to-*cis* isomerization under specific external stimuli.¹ In this study, these two unique structures were combined to synthesize cycloparaphenylenes containing a single azobenzene unit ([1]cycloazobenzene, [1]CAB) and [2]CAB through an oxidation reaction involving Au-complexes. Both molecules exhibit photo- and thermal-isomerization, with [2]CAB demonstrating higher efficiency due to its flexible structure and extra content of azobenzenes. UV-vis spectroscopy reveals that these molecules follow first-order kinetics as temperature increases, resulting in the activation energy of [1]CAB being higher than that of [2]CAB. Furthermore, these cyclic azobenzene molecules hold promise for applications in guest molecule expulsion and rotaxane formation, offering valuable insights for designing molecular mechanical devices based on azobenzene-induced structural deformation.

Keywords: photo/thermal-stimulation, azobenzene, isomerization, macrocycle, Au-complex oxidation

Graphic / Image

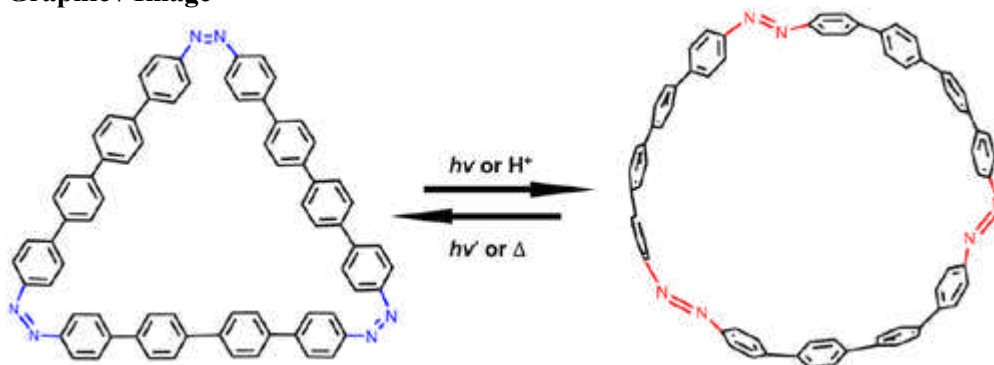


Fig. 1. The schematic illustration of *cis/trans* isomerization of cycloazobenzene.¹

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SYNTHESIS STRATEGIES TOWARD INDIGO ANALOGS

Dyah U. C. Rahayu^a, Stephen G. Pyne^a, Haibo Yu^a, John B. Bremner^a, Jason A. Smith^b,
 Paul A. Keller^{a,*}

^aSchool of Science, University of Wollongong, Wollongong NSW 2522, Australia

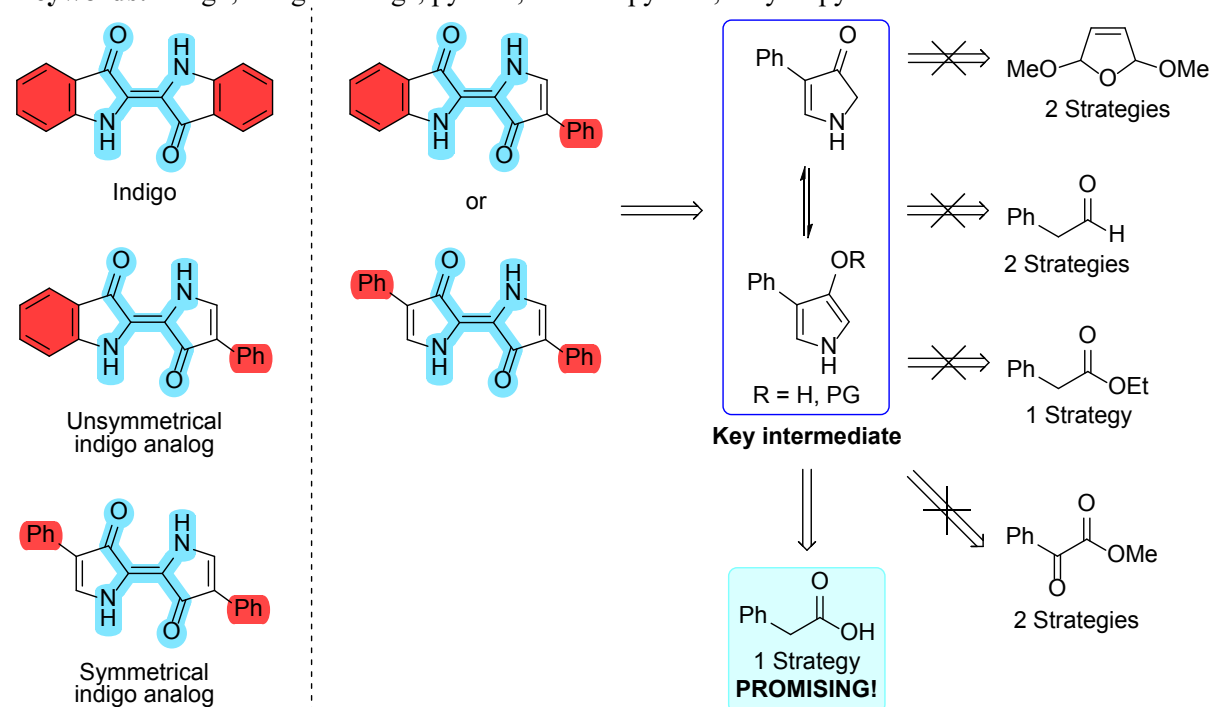
^bSchool of Natural Sciences – Chemistry, University of Tasmania, Hobart TAS 7001, Australia

*Corresponding author: keller@uow.edu.au

Abstract

Indigo, an ancient dark blue dye pigment, is a suitable starting material in complex heterocycle synthesis using one-pot cascade reactions.^{1,2} The chemistry of indigo cascade reactions focuses on the extensively conjugated diamino-diketo-ethylene framework.³ This study aims to synthesize unsymmetrical and symmetrical indigo analogs that retain the reactive central core motifs in the absence of benzene-fused ring(s) for further investigation in cascade reactions. The synthesis of these analogs involves the synthesis of key intermediate, pyrrole or dihydropyrrole. Herein the discussion will be focused on several strategies to generate key intermediate with some alternative oxidation attempts toward indigo analogs. To access the key intermediate, eight synthetic approaches with five different starting materials were devised and attempted, leading to one promising strategy. With this strategy, we successfully synthesized *N*-benzyl-protected dihydropyrrole together with promising access to obtain novel dimeric pyrroles. Various attempts to yield indigo analogs with the computational study will be also discussed.

Keywords: indigo, indigo analogs, pyrrole, dimeric pyrrole, dihydropyrrole



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SYNTHESIS AND *IN SILICO* EVALUATION OF CHALCONE-COUMARIN HYBRIDS AS BACE-1 INHIBITORS FOR POTENTIAL ALZHEIMER'S THERAPY

Nico Andreas^a, Wildan Sahari^a, Muhammad Rifky Chairin^a, Aldi Dwi Febrianto^a, Dyah Utami Cahyaning Rahayu^b, Hanhan Dianhar^{a,*}

^aChemistry Study Program, Faculty of Mathematics and Natural Sciences Universitas Negeri Jakarta, Jakarta, Indonesia

^bDepartment of Chemistry, Faculty Mathematics and Natural Sciences, Universitas Indonesia, Depok, West Java, Indonesia

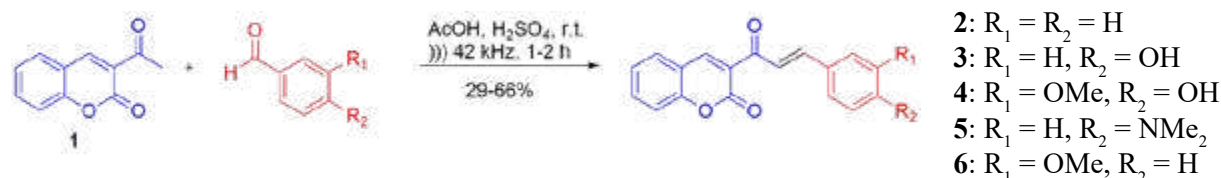
*Corresponding author: hanhan@unj.ac.id

Abstract

Alzheimer's is a disease caused by decreased organ function with aging¹. This disease is ranked sixth as the leading cause of death worldwide in 2023². Amyloid Precursor Protein (APP) plays a major role in the growth and repair of neurons. APP is digested by three main enzymes, namely α -secretase, β -secretase, and γ -secretase into soluble protein fibers. These protein fibers will be digested and reused later. However, in the process of breaking down APP, the β -secretase (BACE-1) can trigger new problems in neurons³. By this cause, inhibition of β -secretase performance is needed to prevent further plaque formation. One of the compounds that has the potential to be an inhibitor of β -secretase are chalcone and coumarin^{4,5}. Many researchers reported chalcone and coumarin derivatives and their BACE-1 inhibitors but the activity of hybrid compounds of them are still limited. Therefore, this research was aimed to synthesize chalcone-coumarin hybrids and evaluate its potential BACE-1 inhibitors by computational study. In this research, the chalcone and coumarin hybrids were obtained by reaction of 3-acetylcoumarin (**1**) and some benzaldehydes by using ultrasound irradiation. The structure of five hybrids (**2-6**) were identified based on UV-vis, ¹H-NMR, and mass spectra. All compounds were evaluated for its potential BACE-1 inhibitor by molecular docking. Hybrid **2** and **5** showed the highest binding affinity due to their strong hydrogen bonds and van der Waals interactions. The activity of the hybrids **2-6** will be further investigated for their inhibitory activity *in vitro*.

Keywords: Alzheimer's, BACE-1, chalcone, coumarin, hybrids

Graphic / Image



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FROM DNA-PROGRAMMED BIOMEMBRANE FUSION TO OLIGONUCLEOTIDE DELIVERY

Kalisi, Nazmie^a, Vogel, Stefan^{a*}

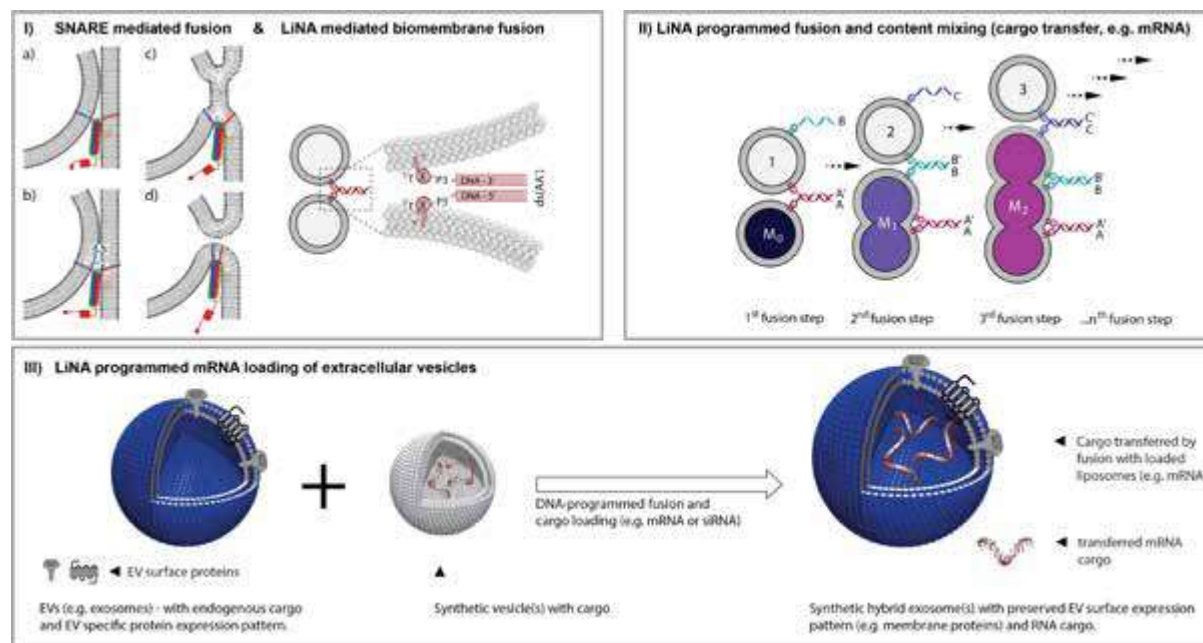
^a*Nucleic Acid Center, Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Campusvej 55, 5230 Odense, Denmark*

**Corresponding author: snv@sdu.dk*

Abstract

The current appreciation of extracellular vesicles (EVs, especially exosomes) as important biological entity with primary tasks in cellular communication and transport of material has changed our understanding of biology. Exosomes are abundant lipid nanoparticles (40-160 nm) in biology which are released and taken up by all cells. Exosomes travel through the body and cross most biological barriers including the blood–brain barrier (BBB). Application of exosomes as an advanced delivery platform would be an enabling technology for therapeutics and oligonucleotides in particular (e.g., siRNA, mRNA). The major obstacles to harvest the enormous potential of this delivery platform are multifold, with a lack of user-friendly tools to isolate, upscale and modify exosomes and no efficient method for loading of cargo into isolated exosomes available. Our unique DNA-programmed biomembrane fusion technology based on lipidated oligonucleotides (LiNAs) enables controlled loading of therapeutic oligonucleotides into exosomes. ^[1-2] The platform presented shows non-viral delivery based on synthetic hybrid exosomes with mRNA encapsulation, fusion of exosomes and delivery to cells.

Keywords: drug delivery, oligonucleotides, biomembrane fusion, lipid nanoparticles



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CONVERSION OF INDANONE-DERIVED GEMINAL AZIDOFUORIDES TO ISOQUINOLINES OR BENZOYL FLUORIDES

Fanhong Wu*, Shixun Liu, Jingjing Wu, Shibo Xu

School of Chemical and Environmental Engineering and Shanghai Engineering Research Center of Green Fluoropharmaceutical Technology
Shanghai Institute of Technology

Shanghai 201418, People's Republic of China

*Corresponding author: wfh@sit.edu.cn

Abstract

In the field of organic chemistry, fluorinated compounds have garnered significant attention due to their unique physicochemical properties and broad application prospects. In recent years, the increasing availability of methods for inserting, deleting, or exchanging single atoms within molecular cores has provided new ideas and approaches for synthesizing novel fluorinated compounds.¹ Nitrogen, as a key element in organic molecules, can modulate the polarity, stability, and reactivity of molecules, while also imparting new functional properties. By incorporating nitrogen atoms into the molecular framework of fluorinated compounds, we can further expand the chemical space, leading to the development of compounds with novel structures and functions.²

In this article, we describe a method for introducing azide groups as a nitrogen source into pre-synthesized monofluorohaloketones. Through selective post-modulation, nitrogen atoms can be readily inserted into monofluoroketones to form entirely new skeleton-fluorinated isoquinolinols. Additionally, by controlling the reaction conditions, fluorine-migrated acyl fluorides can also be synthesized (Fig. 1). This strategy provides a novel pathway for the synthesis of innovative fluorinated compounds. The reaction can be efficiently conducted under open-air conditions, yielding target compounds with high efficiency. Subsequent functionalization of drug molecules and further mechanistic studies will also be included in our presentation.

Keywords: Fluorinated compounds, Skeleton editing, Nitrogen insertion, Fluorine migration

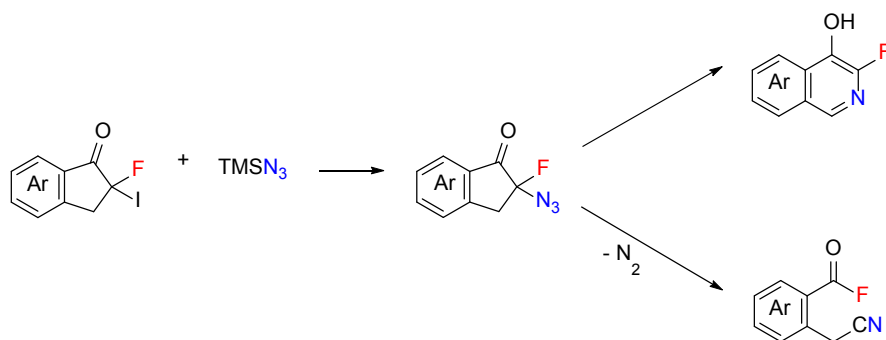


Fig. 1 Conversion of indanone-derived geminal azidofluorides to isoquinolines or benzoyl fluorides

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ON-BEAD AMIDATION FOR THE SITE-SELECTIVE SIDE-CHAIN MODIFICATION

Chai-Lin Kao*, Yi Kai Lin,

*Department of Medicinal and Applied Chemistry,
Kaohsiung Medical University, Kaohsiung 807, Taiwan.*

**Corresponding author: clkao@kmu.edu.tw*

Abstract

The selective modification of a peptide is vital for the biomedical applications of peptides. However, most modification was achieved in liquid-phase, which surrendered the advantage of solid-phase synthesis and created difficulty in handling and purification. We have developed 3,4-diaminobenzate (Dbz) as a safety-catch linker to propagate long peptides, cyclic peptides, branch peptides, and peptidol to accomplish the on-bead modifications.¹⁻³ In preparation, Dbz was used as a stable linker for the solid-phase peptide synthesis (SPPS). Once the designed length of peptides was reached, the treatment of alkyl nitrite gave benzotriazole (Bt), which served as an excellent leaving group for introducing a nucleophile. Herein, 1,2-diamino-4-nitrobenzene (Dnb) was introduced to the side-chain of Asp and Glu residues to prepare the Fmoc-Glu(Dnb)-OH and Fmoc-Asp(Dnb)-OH. Both residues adapted to popular resin and reaction conditions in SPPS. Upon activation, the following acylbenzotriazole is a leaving group for the on-bead introduction of various amines, including aliphatic chains and peptides. Furthermore, the on-bead reduction of acylbenzotriazole gave a hydroxyl group on the side chain. This approach provided a convenient method to introduce various moieties at the designed position.

Keywords: Solid-phase peptide synthesis, side chain modification, diaminonitrobenzene,

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DESIGN AND SYNTHESIS OF INDOLE-BASED ANTIBACTERIAL COMPOUNDS

Chee Wei Ang* Jiwoo Kim, Minghao Qi, Kong Huan Yong, Joo Kheng Goh

^aMonash University Malaysia

*Corresponding author: ang.cheewei@monash.edu

Abstract

Antimicrobial resistance (AMR) is one of the primary global health threats in the 21st century. With increasing resistance to current drugs, there is an urgent need to find new therapeutics to combat the rise of AMR. In this study, we utilize a versatile chemical scaffold, indole^{1,2} as the template to design new antimicrobials. Different series of indole hydrazones were synthesized, and their biological activity against both Gram-positive and Gram-negative bacteria was evaluated. Given the possibility of hydrazones to form configurational isomers due to the carbon-nitrogen double bond,^{3,4} a brief investigation was also performed by exploring their reaction parameters. Among the twenty-two compounds that were synthesized, compound **IN10** displayed the most potent activity (minimum inhibitory concentration of 2-4 µg/mL) across a broad spectrum of bacteria, including methicillin-resistant *Staphylococcus aureus* (MRSA). From the structure-activity relationship, we found that substitution at N-1 position of indole moiety is essential to enhance its antibacterial effect, especially when lipophilic side chain was installed. In summary, our study demonstrates the potential of indole-based derivatives to be developed as lead compounds against resistant pathogens.

Keywords: Antimicrobial resistance, indole, hydrazine, configurational isomerism

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PHARMACOPHORE BASED DESIGNING, SYNTHESIS AND BIO EVALUATION OF HETEROCYCLIC COMPOUNDS AS IMMUNOMODULATING AGENTS

Saima Kalsoom^{a,b,*}, Farzana Latif Ansari^b, Stefano Moro^c, Zaheer-ul-Haq Qasmi^d,
Humaira Masood Siddiqi^b, Ahmed Mesaik^d, Iram Batool^b.

^aDepartment of Chemistry, PMAS-Arid Agriculture University, Rawalpindi, Pakistan

^bDepartment of Chemistry, Quaid-i-Azam University, Islamabad, Pakistan

^cDepartment of Pharmacy, University of Padova, Padova, Italy

^dDr. Pajanjwani Centre for Molecular Medicines & Drug Research, ICBB, University of Karachi, Pakistan.

*Corresponding author: Saimakalsoom@uaar.edu.pk

Abstract

Cytokine Interleukin-2 (*IL-2*) is prevalent in T cells' growth, activation, and differentiation. To suppress immune responses associated with organ transplant rejection and other autoimmune diseases, it is important to disrupt the interaction of *IL-2* with its receptor system. *IL-2* is now emerging as a target in drug discovery for novel therapeutic approaches in several autoimmune disorders. The main goal of this study was to establish an effective *in silico* protocol for the identification of *IL-2* inhibitors. It describes pharmacophore-based virtual screening combined with docking study as a rational strategy for the identification of novel hits as *IL-2* inhibitors. A structure-based pharmacophore model was developed using the crystal structure of the *IL-2/IL-2R α* (PDB ID: 1Z92) complex. Pharmacophore-based molecular docking studies were carried out on all hit compounds by MOE software showing hydrogen bonding, π - π and hydrophobic interactions. Key contributing amino acids observed in the binding pocket of docked complexes were Ile28, Leu36, Phe42, Tyr43, Glu62, Pro63, Val69, Asn71 and Leu72. This combination of *in silico* methodologies is a valuable tool for identifying structurally diverse molecules for *IL-2* inhibition. Later, the designed library of forty-six compounds (including derivatives of Chalcones, Dihydropyrimidines, Pyrazoles, Benzimidazoles, Anthraquinone sulfonamide and Benzamides) was synthesized and characterized by spectroscopic techniques for onward screening for their *IL-2* inhibition assay by using cyclosporine as a standard drug. All were found to be potent inhibitors, able to block *IL-2* production with IC₅₀ values ranging from <2 to >50 μ g/ml. Compounds **1, 2, 4, 5, 7, 11 & 43** were found to possess the most potent inhibitory activity among all with IC₅₀ ranges from <2 to 5.30 μ g/mL. Compounds **31, 35, 39 & 42** were found to have potent *IL-2* inhibitory activity with IC₅₀ values 6.1, 8.9,

3.63 & 3.65 μ g/mL respectively. All remaining compounds showed moderate *IL-2* inhibition activity. This entire set of experiments in both dry and wet labs led to a successful designing and Synthesis of a variety of heterocyclic compounds as a novel scaffold having strong *IL-2* inhibition activities.

Keywords: Heterocyclic compounds, Immunomodulating Agents, Structure Based Pharmacophore, Molecular Docking.

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LIQUID CRYSTALLINE AND FIRE RETARDANT EVALUATION OF NEW CYCLOTRIPHOSPHAZENE DERIVATIVES WITH ESTER-SCHIFF BASE LINKAGES

Zuhair Jamain^{a*}, Nur Atika Waldin^a, Melati Khairuddean^b, Tay Guan-Seng^c

^aOrganic Synthesis and Advanced Materials (OSAM) Research Group, Faculty of Science and Natural Resources, Universiti Malaysia Sabah, Jalan UMS, 88400 Kota Kinabalu, Sabah, Malaysia

^bSchool of Chemical Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia

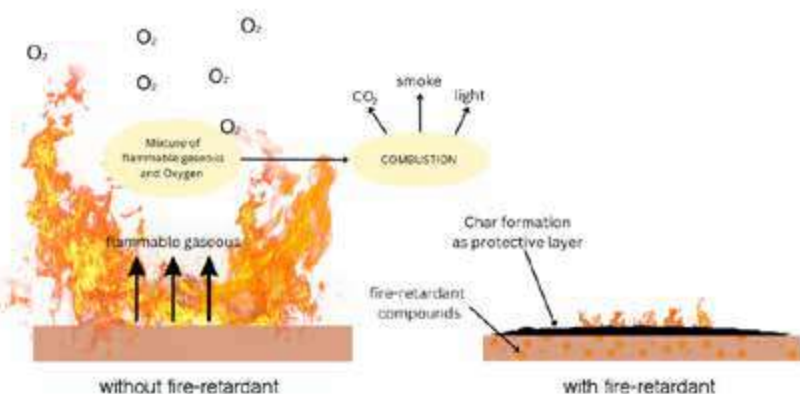
^cSchool of Industrial Technology, Universiti Sains Malaysia, 11800 Penang, Malaysia

*Corresponding author: zuhairjamain@ums.edu.my

Abstract

A series of new hexasubstituted cyclotriphosphazene compounds, featuring ester and Schiff base linkages, were successfully synthesized and characterized. In this series, various terminal substituents, including nonyl, dodecyl, hydroxy, and nitro groups, were incorporated into the side arms of cyclotriphosphazene. The compounds were characterized using organic spectroscopic techniques such as Fourier transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR) spectroscopy, and CHN elemental analysis. Their liquid crystal properties were assessed using polarized optical microscopy (POM), which revealed that all compounds exhibited mesogenic behavior, showing nematic phases during heating and cooling cycles. Differential scanning calorimetry (DSC) further validated these phase transitions, with two endothermic peaks corresponding to the crystal-nematic-isotropic transitions. Moreover, the fire retardancy of the hexasubstituted cyclotriphosphazene compounds was evaluated using the limiting oxygen index (LOI) test, with polyester resin (PE) serving as the matrix. Pure PE exhibited an LOI value of 22.53%, which increased to 24.71% when blended with 1 wt.% hexachlorocyclotriphosphazene (HCCP), indicating significant fire retardant properties. Further modifications of HCCP with organic side chains demonstrated that all compounds exhibited fire retardancy, as evidenced by their LOI values. The compound with a nitro terminal group showed the highest LOI value of 27.53%, suggesting that the electron-withdrawing nature of the nitro group and the ester-Schiff base linkages played a crucial role in enhancing the fire retardant performance.

Keywords: cyclotriphosphazene; ester-Schiff base; liquid crystals; fire retardancy; nitro group



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PURITY DETERMINATION OF CAFFEINE AS HIGH-PURITY ORGANIC SUBSTANCE REFERENCE MATERIAL USING A MASS BALANCE APPROACH

Nor Fariha Muhamad Zin^{a,*}, Haznita Rose Bahari^a, Dr Siti Nur Nazathul Shima Hashim^a,

^aChemical Metrology Division, Department of Chemistry Malaysia, Petaling Jaya, Selangor, Malaysia.

**Corresponding author: norfariha@kimia.gov.my*

Abstract

The study aimed to evaluate the purity of caffeine, the primary stimulant in coffee and tea, as a high-purity organic reference material. The purity assessment was conducted using a mass balance approach in accordance with ISO 17034:2016 and ISO Guide 35:2017 for reference material production. Homogeneity testing, performed via High-Performance Liquid Chromatography (HPLC) and supported by statistical analysis, confirmed substance uniformity. Impurities, including those from structurally related organic compounds, residual organic solvents, and non-volatile residues, were analyzed using HPLC, Karl Fischer Coulometry, and Thermogravimetric Analysis (TGA) respectively. The determined purity was found to be $99.08\% \pm 0.69\%$. Stability testing was conducted over four years and confirmed the material's suitability as reference material for caffeine analysis.

Keywords: caffeine, reference material, mass balance

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SYNTHESIS AND ANTIMALARIAL EVOLUTION OF TRANSITION METAL SCHIFF BASE AND DIRHODIUM(II) COMPLEXES WITH 4-AMINOQUINOLINE SCAFFOLDS

Nurul Izzaty Hassan^{a,*}, Nur Aqilah Zahirah Norazmi^a, Ravindar Lekkala^a, Nurul Huda Abd Karim^a, Wan Nurfadhilah Zaharim^a, Lau Yee Ling^b, Fazira Ilyana Abdul Razak^c, Hani Kartini Agustar^d, Saki Raheem^e, Nurzila Ismail^f & Masahiro Ebihara^g

^aDepartment of Chemical Sciences, Faculty of Science & Tehcnology, UKM

^bDepartment of Parasitology, Faculty of Medicine, UM; ^cDepartment of Chemistry, Faculty of Science, UTM;

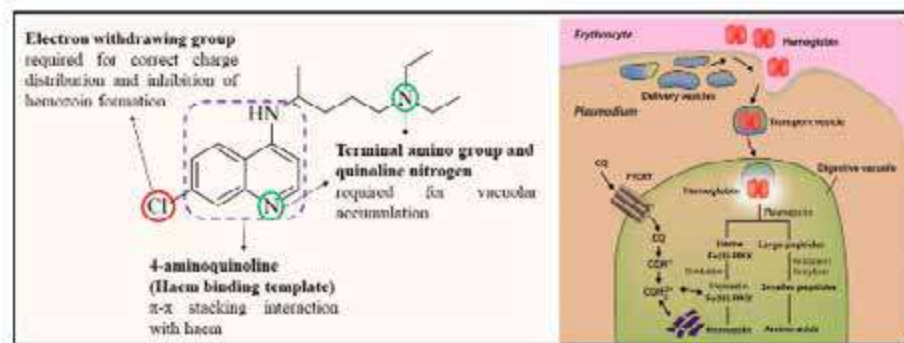
^dDepartment of Biological Sciences and Biotechnology, Faculty of Science & Tehcnology, UKM; ^eSchool of Life Sciences, University of Westminster, 115 New Cavendish Street, W1W 6 UW, London, UK; ^fDepartment of Pharmacology, School of Medical Sciences, USM; ^gDepartment of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University, 1-1 Yanagido, Gifu City 501-1193, Japan

*Corresponding author: drizz@ukm.edu.my

Abstract

Malaria, transmitted by Anopheles mosquitoes, remains a global health threat, exacerbated by rising resistance to antimalarial drugs like artemisinin. This paper aims to develop and evaluate transition metal complexes with established antimalarial pharmacophores, such as 4-aminoquinoline, a key component in chloroquine. Building on the success of ferroquine, a series of Schiff base salphen ligands **1-6** with various substituents (H, F, Cl, Br, COOH, and NO₂) and their corresponding Ni(II) complexes **7-12** were synthesized and characterized. After an initial attempt to conjugate salphen ligands with 4-aminoquinoline was unsuccessful, a salicylaldimine Schiff base ligand **13** linked to a 4-aminoquinoline scaffold was successfully synthesized, resulting in a series of Ni(II), Cu(II), and Zn(II) complexes **14-19** with different metal-ligand ratios (1:1 and 1:2). Additionally, dirhodium(II) tetraacetate complexes incorporating 4-aminoquinoline via the quinoline nitrogen **25-29** were synthesized to explore the potential of dirhodium(II) complexes as novel antimalarial agents. All ligands and complexes were characterized using Nuclear Magnetic Resonance (NMR) and Fourier Transform Infrared Spectroscopy (FT-IR) and evaluated in vitro against chloroquine-sensitive 3D7 and chloroquine-resistant K1 Plasmodium falciparum strains. In the salphen series, although none of the compounds surpassed chloroquine diphosphate (CQDP) in potency, their resistance indices were superior, with halide-substituted compounds showing the highest activity—ligand **3** (Cl) against 3D7 and complex **8** (Cl) against K1. Most Ni(II) complexes exhibited improved activity over their corresponding ligands, except for complexes **11** and **12**, which showed reduced activity. In the salicylaldimine-aminoquinoline Schiff base series, all compounds showed potent activity against the 3D7 strain and outperformed CQDP against the K1 strain. The dirhodium(II) tetraacetate series compounds **28** and **29** demonstrated promising activity, particularly against the K1 strain. The most promising candidates were found in the salicylaldimine series **13-19**, with IC₅₀ values ranging from 0.01-0.09 μ M (3D7) and 0.02-0.19 μ M (K1), supported by excellent ADMET properties, suggesting their potential as drug candidates for further antimalarial development.

Keywords: Schiff base, Salphen, 4-aminoquinoline, malaria, dirhodium (II) tetraacetate



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CYCLOADDITION REACTIONS: EXPERIMENTAL AND COMPUTATIONAL APPROACHES

Lydia Rhyman^{a,b*}, Ponnadurai Ramasami^{a,b}

^a*Computational Chemistry Group, Department of Chemistry, Faculty of Science, University of Mauritius, Réduit 80837, Mauritius.*

^b*Centre For Natural Product Research, Department of Chemical Sciences, University of Johannesburg, Doornfontein, Johannesburg, 2028, South Africa.*

**Corresponding author: lyd.rhyman@gmail.com*

Abstract

Cycloaddition reactions are atom-efficient processes which are widely used in the synthesis of carbo- and heterocycles. The most common types of cycloaddition reactions are the Diels-Alder and the 1,3-dipolar cycloaddition reactions leading to the formation of six- and five-membered ring systems, respectively. Their versatile reactivity has opened up new avenues for the synthesis of a variety of building blocks as their products are the backbones of many complex natural products. It is important to understand the mechanism of cycloaddition reactions so that reaction conditions can be optimised for synthesis, particularly to rationalise the regio- and stereochemistry of these reactions. However, the mechanism through which the cycloaddition reactions occur makes it difficult to elucidate experimentally but can be fully addressed using computational methods. In this presentation, we will provide an overview of our contributions in the understanding of cycloaddition reactions over the past 15 years.¹⁻³

Keywords: cycloaddition reaction, Diels-Alder, 1,3-dipolar cycloaddition, computational chemistry method

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DEVELOPMENT OF CARBOHYDRATE-BASED DRUGS AND PRODRUGS TO OVERCOME ANTIMICROBIAL RESISTANCE

Catarina Maria^{a,*}, Amélia P. Rauter^a, Rodrigo F. M. de Almeida^a, Nuno M. Xavier^b,

^a*Centro de Química Estrutural, Institute of Molecular Sciences, University of Lisbon.*

^b*Med.Ulisboa*

*Corresponding author: cbmaria@fc.ul.pt

Abstract

Antimicrobial resistance (AMR) is recognized by the World Health Organization (WHO) as one of the top ten health threats. Bacterial AMR is a concerning phenomenon due to the rapid emergence of the widely spread multidrug-resistant bacteria [1,2]. Gram-negative bacteria (GNB) are particularly concerning, and in 2024, WHO published the list of priority pathogens divided into three groups, amongst which the most critical one is composed exclusively of GNB resistant strains [3].

In the last decades, our Carbohydrate Chemistry Group (CCG) has been dedicated to the development of antibacterial carbohydrate-based agents, having obtained promising results with alkyl deoxyglycosides, which have been synthesized and extensively studied [4-8]. In this context, dodecyl deoxyglycosides have shown potent activity against Gram-positive bacteria strains, namely *Bacillus cereus* and *Bacillus anthracis*. The mode of action of deoxyglycosides is related to their interaction with membrane phosphatidylethanolamine lipids. However, the outer membrane (OM) of GNB prevented compounds from reaching inner membrane and exhibit antibacterial effects [4-7]. The repurposing of the previously studied class of compounds against GNB started in 2024 by CCG through two main strategies: The prodrug strategy and the combination approach. The latter started with combination of dodecyl deoxyglycosides with sub-therapeutical concentrations of polymyxins, leading to promising results against drug-resistant GNB strains included in the WHO critical priority group [8]. The prodrug approach is currently under development, with the synthesis of disaccharides mimicking the GNB cell wall *N*-acetyl muramic acid-*N*-acetylglucosamine (MurNAc-GlcNAc) repeat unit. These mimetics, bearing a dodecyl glycoside linked to a MurNAc unit, are expected to cross OM, be hydrolyzed by GNB intrinsic lysozymes, and release the dodecyl glycoside unit to interact with the inner membrane and promote antibacterial effects.

With these new strategies we aim at contributing to the research in the field of overcoming the concerning phenomenon of AMR.

Keywords: Antimicrobial Resistance; Drug Development; Carbohydrate Chemistry; Organic Chemistry; Medicinal Chemistry

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HYPERBARIC SYNTHESIS OF CYCLOBUTANE LIBRARIES FOR FRAGMENT-BASED DRUG DISCOVERY

Daniel Blanco-Ania^{a,*}, Mathilde A. C. H. Janssen^a, Floris P. J. T. Rutjes^a

^aInstitute for Molecules and Materials, Radboud University Nijmegen

*Corresponding author: daniel.blancoania@ru.nl

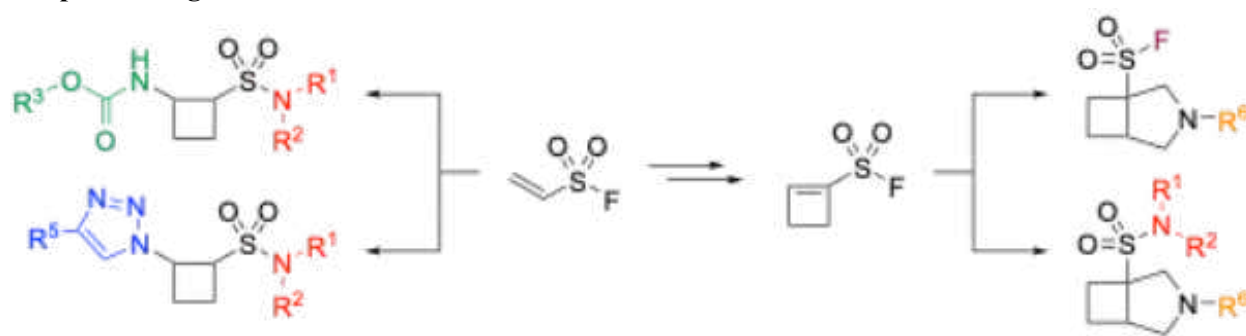
Abstract

This presentation explores the synthesis of disubstituted monocyclic and bicyclic cyclobutane libraries for fragment-based drug discovery (FBDD). Over the past 25 years, FBDD has become a well-established approach in medicinal chemistry for generating lead compounds,¹ leading to the discovery of seven FDA-approved drugs. The incorporation of three-dimensional fragments into fragment libraries has gained increasing interest because of their potential advantages over flat aromatic fragments, including improved solubility, pharmacokinetic properties, and structural diversity. In this context, cyclobutanes—characterized by structural rigidity and stereochemical complexity—have emerged as underrepresented yet promising 3D scaffolds in FBDD.² Their unique properties, such as conformational restriction, can enhance pharmacological activity and drug-like characteristics.

The synthetic approach to the aforementioned libraries was initiated using hyperbaric [2+2] cycloaddition reactions with ethenesulfonyl fluoride and 1,3-dipolar cycloadditions with cyclobutene-1-sulfonyl fluoride, yielding cyclobutanesulfonyl fluoride and 3-azabicyclo[3.2.0]heptane-1-sulfonyl fluoride derivatives, respectively. The monocyclic cyclobutanesulfonyl fluoride derivatives were subsequently diversified into small libraries of sulfonamides, carbamates, and triazoles.³ Likewise, the bicyclic derivatives underwent further functionalization, enabling the generation of both covalent and non-covalent compound libraries through various derivatization strategies. In total, we synthesized more than 80 novel cyclobutane derivatives using parallel synthesis techniques.

Keywords: Fragment-based drug discovery, cyclobutanes, high-pressure synthesis, library synthesis, parallel synthesis

Graphic / Image



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BIOCATALYTIC PROTEIN MODIFICATION FOR THE DEVELOPMENT OF NEXT-GENERATION THERAPEUTIC AGENTS

Mark D. Distefano,^{a,*} Yiao Wang^a, Sneha Venkatachalapathy^a,
Mohammad Rashidian,^b Carston R. Wagner^a

^aUniversity of Minnesota

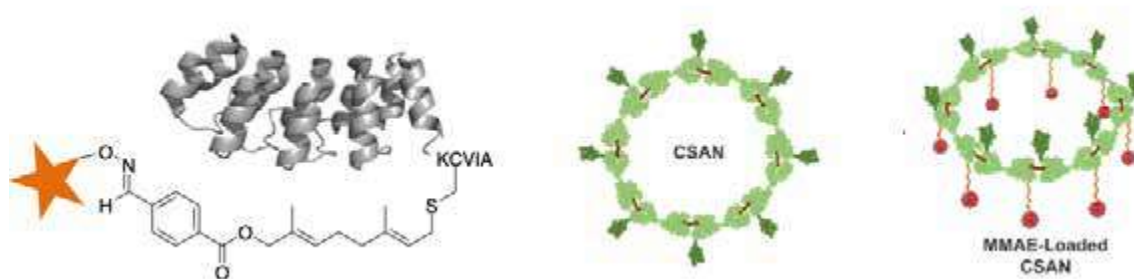
^bHarvard Medical School

*Corresponding author: diste001@umn.edu

Abstract

Protein-based drugs, also known as biologics, are becoming more prevalent as therapeutic agents. Many of these molecules involve the attachment of various small molecules including cytotoxic agents or metal-chelating groups to proteins. To date, chemical modification of lysine and cysteine residues has been the primary method for preparing protein conjugates. However, such methods have important limitations in terms of specificity and stability. In the last 10 years, numerous enzymatic methods have been developed that allow highly selective protein modification.¹ Using farnesyltransferase, we have shown that substrate analogues containing functionality including, aldehydes, alkynes, azides and strained alkenes can be enzymatically incorporated with high efficiency into proteins. Subsequent biorthogonal ligation reactions afford proteins with unique reactive chemical handles that can be exploited for subsequent protein derivatization.² Examples of proteins linked to cytotoxic natural products for targeted cancer cell killing and proteins incorporating metal ion chelators for PET imaging will be discussed. Enzymatic incorporation of natural and modified prenyl groups has also been used to construct macromolecular protein assemblies with novel properties that can be used for a variety of purposes. Farnesylation of chemically self-assembling nanorings (CSANs) has allowed the creation of multimeric protein structures that bind with high affinity to cell surfaces. Those molecules can be further decorated with additional cargos using bioorthogonal chemistry. The use of modified CSANs for cell killing, imaging and cellular barcoding will be presented. It should be noted that all of proteins used in the aforementioned experiments were produced via bacterial expression, avoiding the use of heterogeneous and expensive antibodies. The use of non-antibody scaffolds combined with efficient biocatalytic methods for selective modification described here should increase the utility and decrease the cost of the next generation of protein-based drugs.

Keywords: biocatalysis, farnesyltransferase, prenylation, protein modification, protein therapeutics



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TANDEM [4+2] CYCLOADDITION REACTION FOR DIVERSE FUSED TETRAHYDROPYRIDINE SCAFFOLDS

Xiuyu Chen, Chao-Guo Yan*

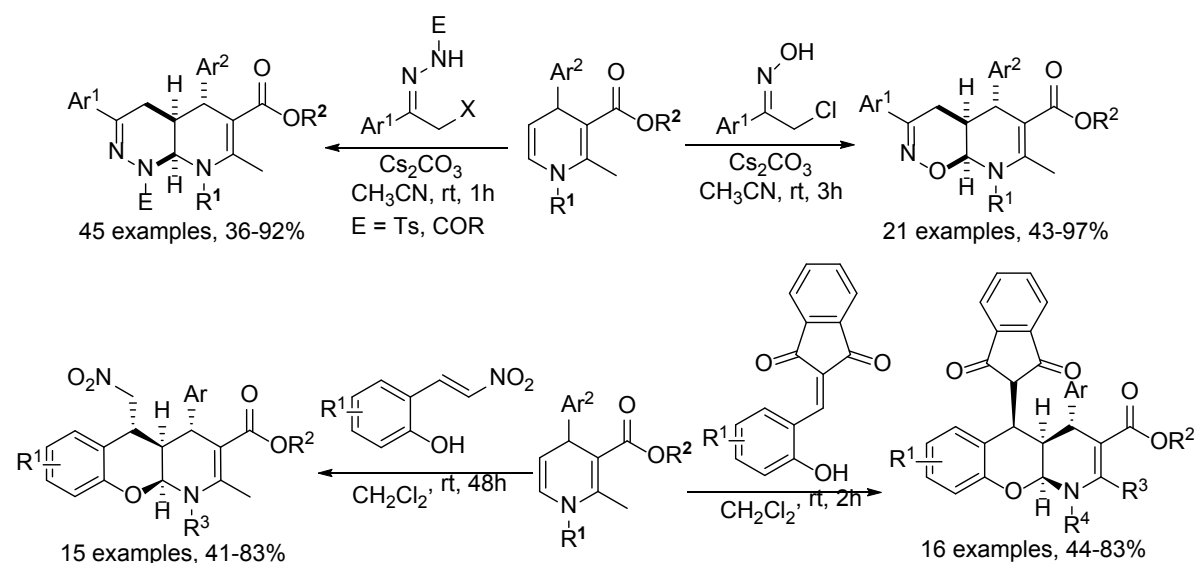
College of Chemistry & Chemical Engineering, Yangzhou University, Yangzhou 225002, China

*Corresponding author: cgyan@yzu.edu.cn

Abstract

A convenient synthetic protocol for diverse fused tetrahydropyridine derivatives with excellent regioselectivity and diastereoselectivity was successfully developed by tandem [4+2] cycloaddition reaction. The functionalized pyrido[2,3-*c*]pyridazines were successfully synthesized via Cs_2CO_3 promoted [4+2] cycloaddition reaction of α -halogenated *N*-tosylhydrazones or *N*-acylhydrazones and 5,6-unsubstituted 1,4-dihydropyridines under mild conditions. Additionally, the similar base promoted [4+2] cycloaddition reaction of α -chlorogenated oximes and 5,6-unsubstituted 1,4-dihydropyridines afforded functionalized pyrido[3,2-*e*][1,2]oxazines in satisfactory yields. In addition, the functionalized chromeno[2,3-*b*]pyridines were efficiently synthesized by [4+2] cycloaddition reaction of 2-(2-nitrovinyl)phenols or 2-(*o*-hydroxyarylidene)-1,3-indanediones and 5,6-unsubstituted 1,4-dihydropyridines at room temperature in the absence of any catalyst. The features of this reaction included mild reaction conditions, broad substrate scopes, high functional group tolerance and significant atomic economy.

Keywords: α -halogenated *N*-tosylhydrazone; 1,4-dihydropyridine; pyrido[2,3-*c*]pyridazine; pyrido[3,2-*e*][1,2]oxazine; [4+2] cycloaddition.



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NATURAL PRODUCT-INSPIRED THIOSEMICARBAZONES: SYNTHESIS, *IN VITRO* ANTI-MALARIAL ACTIVITY, ANTIPROLIFERATIVE ACTIVITY AND *IN SILICO* MOLECULAR DOCKING AND MOLECULAR DYNAMIC SIMULATION STUDIES

Ming Yueh Tan^{a*}, Sheng Zhou Ho^a, Hui Yin Tan^a, Siow Ping Tan^a, Siew Lee Cheong^b, Yee Ling Ng^c

^aDepartment of Physical Science, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Kelang, Setapak, 53300 Kuala Lumpur, Malaysia.

^bDepartment of Pharmaceutical Chemistry, School of Pharmacy, International Medical University, No. 126, Jalan Jalil Perkasa 19, Bukit Jalil, Kuala Lumpur 57000, Malaysia.

^cDepartment of Parasitology, Universiti of Malaya, 50603 Kuala Lumpur, Malaysia.

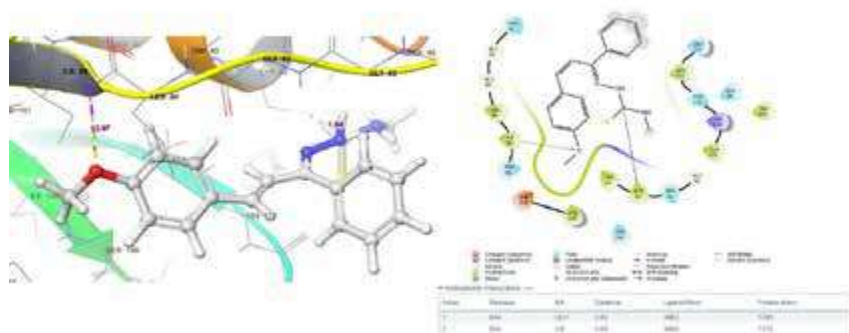
*Corresponding author: tanmy@tarc.edu.my

Abstract

The persistent threat of drug-resistant *Plasmodium* parasites underscores the urgent need for novel antimalarial agents. In this study, a series of natural product-inspired thiosemicarbazones were synthesized and evaluated for their antimalarial activity against the chloroquine-sensitive *P. falciparum* strain (3D7), cytotoxicity in human fibroblast (MRC-5) normal cells, and binding interactions through *in silico* molecular docking and molecular simulations dynamic studies.

The compounds exhibited potent antimalarial activity, with IC₅₀ values ranging from 15.31 to 51.02 μM in the schizont maturation assay. Notably, the *N*-phenyl derivatives displayed significantly higher efficacy than their *N*-methyl counterparts. Importantly, all compounds were non-cytotoxic to MRC-5 cells at concentrations up to 200 μM , demonstrating selective antimalarial action.

To unravel the mechanistic basis of their activity, molecular docking studies were conducted using the falcipain-2 (3BPF) crystal structure. The results revealed that the phenyl ring of the *N*-phenyl thiosemicarbazide scaffold engages in critical hydrophobic interactions with residues in the catalytic triad of falcipain-2, likely contributing to its enhanced inhibitory potency. These findings provide a structural foundation for optimizing thiosemicarbazone-based antimalarial agents with improved selectivity and efficacy.



SYNTHESIS AND EVALUATION OF THE ANTICANCER ACTIVITY OF *TEUCRIUM POLIUM* FUNCTIONALIZED SILVER NANOPARTICLES AGAINST COLORECTAL CANCER CELLS

Rahma Haitham Ali^a, Mak Kit Kay^b, Pang Jia Chern^a, Mallikarjuna Rao Pichika^c
Anjani Uma Rani Wunnava^{d*}

^a*School of Postgraduate Studies, IMU University, 126, Jalan Jalil Perkasa 19, Bukit Jalil, 57000, Kuala Lumpur, Malaysia.*

^b*Department of Pharmaceutical Chemistry, School of Pharmacy, IMU University, 126, Jalan Jalil Perkasa 19, Bukit Jalil, 57000, Kuala Lumpur, Malaysia.*

^c*Faculty of Medical Sciences, Newcastle University Medicine Malaysia, Jalan Sarjana 1, Educity, 79200 Iskandar Puteri, Johor, Malaysia.*

^d*Centre for Analytical and Pharmaceutical Services, Institute for Research, Development and Innovation, IMU University, 126, Jalan Jalil Perkasa 19, Bukit Jalil, 57000, Kuala Lumpur, Malaysia.*

**Corresponding author: anjaniumarani@imu.edu.my*

Abstract

This study evaluates the anticancer efficacy of *Teucrium polium* functionalized silver nanoparticles (AgNPs), leveraging the plant's documented antioxidant¹, anti-inflammatory², and antimicrobial³ properties. Ethanolic and aqueous extracts were prioritized based on total phenolic (TPC: 140.2 ± 2.4 and 107.2 ± 1.8 mg GAE/g, respectively) and flavonoid content. The hexane extract with negligible phenolic content was not explored further. Phytochemical profiling of the plant extracts via UV-Vis, FTIR, LC-MS, and HPLC identified dominant bioactive constituents, including terpenoids and flavonoids linked to anticancer activity. Green synthesis of AgNPs was optimized at 10 mg/mL extract concentration, pH 10.5, and 4-hour incubation period, yielding nanoparticles (≤ 130 nm) with enhanced surface reactivity. Cytotoxicity screening revealed concentration-dependent selectivity: ethanolic AgNPs reduced Caco-2 colorectal cancer cell viability to $11.15 \pm 0.69\%$ at 10 $\mu\text{g/mL}$, while sparing CCD-841 normal colon cells ($58.54 \pm 2.98\%$ viability). Dose-response analysis demonstrated low toxicity at 0.3125 $\mu\text{g/mL}$ (Caco-2: $59.79 \pm 1.62\%$; CCD-841: $92.11 \pm 0.95\%$), suggesting a therapeutic window for malignant vs. healthy tissues. The 4.3-fold selectivity index (IC_{50} Caco-2: 2.1 $\mu\text{g/mL}$; CCD-841: 9.0 $\mu\text{g/mL}$) underscores tumour-specific targeting. These findings position *T. polium*-AgNPs as promising candidates for targeted chemotherapy, warranting further investigation into in vivo efficacy and molecular pathways.

Keywords: Phytogetic nanoparticles, colorectal cancer, green synthesis, cytotoxicity, bioactive synergism

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THE BULL-JAMES ASSEMBLY: EFFICIENT IMINOBORONATE COMPLEX FORMATION FOR CHIRAL DERIVATIZATION AND SUPRAMOLECULAR ASSEMBLY

Steven D. Bull

School of Chemistry, University of Leicester, University Road, Leicester, UK

**Corresponding author: sdb45@leicester.ac.uk*

Abstract

Chiral molecules are widely used in many fields of research and so practically simple, accurate methods to measure their enantiopurities are required. This presentation will describe one such method, the Bull-James assembly, which employs a three-component protocol combining 2-formylphenyl boronic acid, an amine, and a diol to self-assemble diastereomeric iminoboronate ester (IBE) complexes whose ratio can be used to measure the *ee*'s of amine and diol analytes using ^1H and ^{19}F NMR spectroscopic analysis.¹ Examples where this supramolecular IBE assembly approach has been used to determine the *ee* of a range of chiral analytes (e.g., amino alcohols, diamines, hydroxylamines, sulfonamides) and use of other analytical techniques such as circular dichroism, fluorescence, and electrochemistry that are potentially applicable to high-throughput *ee* analysis will be discussed.¹



Keywords: Three-Component Complexation, Iminoboronate Ester, Enantiomeric Excess, ^1H and ^{19}F NMR Spectroscopy, Biomolecule Functionalization.

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SYNTHESIS AND ANTICANCER EVALUATION OF NOVEL N^2,N^9 -BENZYLATED- β -CARBOLINEUM BROMATE DERIVATIVES

Mazlin Mohideen^{a,c,*}, Nur Azzalia Kamaruzaman^b, Mohd Nizam Mordic, Sharif Mahsufi Mansor^c

^aFaculty of Pharmacy and Health Sciences, Universiti Kuala Lumpur – Royal College of Medicine Perak (UniKL-RCMP), 30450 Ipoh, Perak, Malaysia.

^bNational Poison Centre, Universiti Sains Malaysia (USM), 11800 Minden, Pulau Pinang, Malaysia.

^cCentre for Drug Research (CDR), Universiti Sains Malaysia (USM), 11800 Minden, Pulau Pinang, Malaysia.

*Corresponding author: mazlin.mohideen@unikl.edu.my

Abstract

Peganum harmala L. is a medicinal plant traditionally used since ancient times due to its alkaloids rich in β -carbolines. Norharman is a naturally occurring β -carboline extracted from *P. harmala* L. that exhibits a wide range of biological, psychopharmacological and toxicology actions. In this study, ten novel β -carboline derivatives consisting of various aldehyde moieties at the C-1 position were synthesized from L-tryptophan via base-catalyzed reactions, followed by N^2,N^9 -benzylated using various benzyl bromides. The prepared compounds were evaluated for *in vitro* cytotoxicity against Hela, HT-29, Hep G2 and K562 cell lines using a 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assay or MTT assay. N^2,N^9 -benzylated- β -carbolineum bromate derivatives **5a-e** exerted promising anticancer activities compared to N^2 -benzylated- β -carboline derivatives, **4a-e**. with compound **5c** exhibited a broad spectrum of activity with an IC_{50} value lower than 20 μ M against all the tested cancer cell lines. Additionally, all β -carboline derivatives displayed moderate antibacterial activities against tested bacterial strains. These findings highlight the potential of N^2,N^9 -benzylated- β -carbolineum bromates as promising anticancer agents.

Keywords: L-Tryptophan, β -carboline, N^2,N^9 -benzylated- β -carboline derivatives, Anticancer activity.

SYNTHESIS, CRYSTAL STRUCTURE AND MOLECULAR DOCKING OF COUMARIN- FUNCTIONALISED N-HETEROCYCLIC CARBENE LIGANDS

Puvana Devi Selvarajoo^{a,b,*}, Mohd Rizal Razali^a, Vikneswari Perumal^{b,c}

^a*School of Chemical Sciences, Universiti Sains Malaysia, Penang, Malaysia.*

^b*Faculty of Pharmacy and Health Sciences, Royal College of Medicine Perak, Universiti Kuala Lumpur, 30450 Ipoh, Perak, Malaysia.*

^c*School of Pharmacy, Management and Science University, Seksyen 13, 40100 Shah Alam, Selangor, Malaysia.*

**Corresponding author: puvana@unikl.edu.my*

Abstract

Structurally and electronically of coumarin and methyl-substituted N-heterocyclic carbene (NHC) ligands derived from benzimidazole core have been prepared and characterized. The ionic salts have been prepared by the successive N-alkylation method using methyl bromide and appropriately 3- bromo(acetyl) coumarin. Structures of ionic salts (1) were established based on elemental analysis, ¹H NMR, ¹³C NMR, IR and CHN techniques. Based on ¹H NMR spectra for salts 1, the characteristic sharp singlet in the range of δ 9.10–9.32 was assigned for acidic proton (NCHN) indicates the successful formation of the targeted ligands. Furthermore, the structure of benzimidazolium salt has been established by single-crystal X-ray diffraction technique. The ionic salt 1 crystallizes in the monoclinic space group P2₁/C, with half of the molecule in the asymmetric unit. The presence of hexafluorophosphate anions in the lattice balances the entire charge of the molecule. Molecular docking studies were carried out to understand the binding interaction of the compound with the active sites of the enzyme.

Keywords: benzimidazole, coumarin, single crystal, carbene, molecular docking

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BENZYLIDENE-HYDRAZONES AS TELOMERASE-TARGETING ANTICANCER AND ANTIOXIDANT AGENTS: SYNTHESIS, CRYSTAL STRUCTURE, PHARMACOKINETIC PROFILING, AND MOLECULAR DOCKING

Mohammad Sayed Alam*

Department of Chemistry, Jagannath University, Dhaka 1100, Bangladesh

*Corresponding author: msalam@chem.jnu.ac.bd

Abstract

Cancer remains one of the most devastating diseases and a major global health concern. Telomerase, a highly specialized reverse transcriptase (RT), represents a promising therapeutic target in anticancer drug development. In this study, a series of benzylidene-hydrazone derivatives (**3a–o**), structurally analogous to known telomerase inhibitors, were synthesized and evaluated for cytotoxicity and antioxidant activity.

The primary aim was to synthesize benzylidene-hydrazone derivatives and evaluate their anticancer activity against four cancer cell lines and antioxidant properties as potential telomerase inhibitors. *In silico* molecular docking was conducted using the crystal structure of the TERT catalytic subunit. Additionally, ADME properties, toxicity profiles, and drug scores were predicted.

Benzylidene-hydrazones (**3a–o**) were synthesized *via* a two-step condensation and characterized by ¹H NMR, mass spectrometry, and single-crystal XRD. Cytotoxicity was evaluated against A549 (lung), SK-OV-3 (ovarian), SK-MEL-2 (skin), and HCT15 (colon) cancer cells using the sulforhodamine-B (SRB) assay. *In silico* ADME, toxicity, and molecular docking studies were conducted using Osiris Cheminformatics and AutoDock Vina.

X-ray analysis of compound **3g** confirmed a tetragonal crystal system (space group I4₁/a) with an *E*-configuration at the azomethine bond. Intermolecular hydrogen bonding involved –NH/–OH donors and >C=O/–N= acceptors. Compound **3e**, bearing two methoxy groups, showed potent cytotoxicity across all cell lines (IC₅₀: 0.024–0.12 μM), comparable to doxorubicin. Compounds **3f**, **3i**, and **3g** demonstrated strong antioxidant activity (IC₅₀: 0.60–1.30 μM), approaching that of ascorbic acid (IC₅₀ = 0.87 μM). All compounds satisfied Lipinski's and Veber's rules, with higher drug scores than doxorubicin and BIBR1532. Docking studies showed strong correlations between binding energies and cytotoxic potency (pIC₅₀), supporting their potential as telomerase-targeting agents.

The synthesized benzylidene-hydrazones, particularly compound **3e**, exhibited significant anticancer and antioxidant activities, with favorable pharmacokinetic profiles. These findings support their potential as telomerase-targeted anticancer agents and justify further *in vivo* investigations.

Keywords: benzylidene-hydrazones, antitumor agents, antioxidant, *In silico* screening, telomerase inhibitor

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OXIDATIVE CYCLIZATION VIA NITROSONIUM IONS

Ahmad Saifuddin Mohamad Arshad^{a,*}, Mohd Nizam Mordi^a

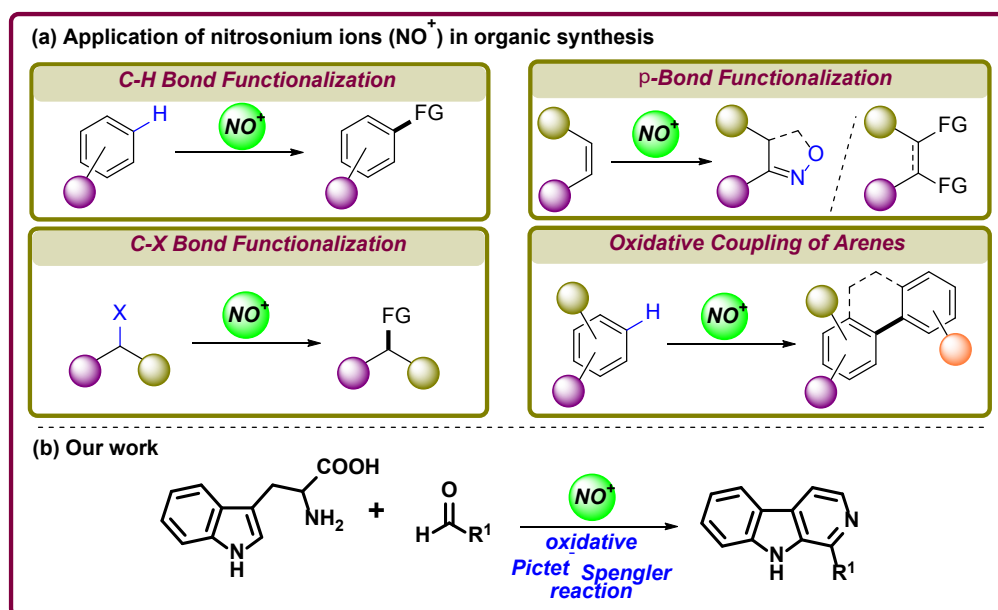
^aCentre for Drug Research, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

*Corresponding author: saifudin_pudin@yahoo.com

Abstract

Nitrosonium ions are non-toxic, stable, and cost-effective single-electron oxidants that have found widespread application across diverse areas of organic synthesis. Their remarkable ability to activate a broad spectrum of substrates through distinct mechanistic pathways enables the catalytic formation of carbon–carbon and carbon–heteroatom bonds, the functionalization of unsaturated systems, and the oxidative coupling of arenes.¹ This versatility positions nitrosonium ions as a promising reagent to tackle current challenges in organic chemistry, facilitating more efficient and sustainable synthetic routes. In this work, we explore the application of nitrosonium ions in oxidative cyclization reactions. We selected the Pictet–Spengler reaction, a pivotal transformation prevalent in natural product biosynthesis, as a model system to demonstrate this concept. While the classical Pictet–Spengler reaction commonly results in non-aromatic cyclized products, exemplified by tetrahydro- β -carboline scaffolds,² our synthetic conditions facilitate an oxidative variant, yielding fully aromatic β -carbolines.³ This biomimetic transformation is reminiscent of the marinacarboline biosynthetic pathway, where enzymatic catalysis constructs the β -carboline framework.⁴ Mechanistic studies suggest a sequence involving tetrahydro- β -carboline formation, followed by decarboxylation and C-ring oxidation to yield the aromatic β -carbolines. Conclusively, our work demonstrates the efficacy of nitrosonium ions in enabling oxidative Pictet–Spengler reactions to access aromatic β -carbolines under mild conditions, offering a novel biomimetic approach.

Keywords: nitrosonium ions, oxidative cyclization, Pictet–Spengler reaction, β -carbolines



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SYNTHETIC APPROACHES TOWARDS BIOACTIVE DAIBUCARBOLINE A DERIVATIVES WITH DUAL ANTI-INFLAMMATORY AND ANTICANCER POTENTIAL FOR NEXT-GENERATION THERAPEUTICS

Noor Hidayah Pungot^{a,b,*}, Nur Ain Nabilah Ash'ari^b, Nur Akmalazura Jani^c, Muhd Hanis Md Idris^b

^aOrganic Synthesis Laboratory, Institute of Science, Universiti Teknologi MARA, Puncak Alam Campus, 43200 Bandar Puncak Alam, Selangor, Malaysia.

^bFaculty of Applied Sciences, Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia.

^cFaculty of Applied Sciences, Universiti Teknologi MARA Kuala Pilah, 72000 Kuala Pilah, Negeri Sembilan, Malaysia.

*Corresponding author: noorhidayah977@uitm.edu.my

Abstract

β -Carbolines are a class of indole alkaloids originally isolated from *Peganum harmala*, known for their rigid heterocyclic structure and diverse pharmacological activities. These include neuroprotective, antioxidant, and antimicrobial properties such as anticancer, antibacterial, antiviral, antimalarial, and anti-HIV effects. Among them, daibucarboline A has demonstrated notable anti-inflammatory potential, particularly with an IC_{50} value of 18.41 μ M in iNOS assays. However, reports on its chemical synthesis remain scarce, and studies on the isolated compound are limited. This study aimed to develop a novel synthetic route for Daibucarboline A and its analogues, targeting compounds with promising anti-inflammatory and anticancer activities. The synthetic strategy involved the preparation of tetrahydro- β -carboline intermediates via Pictet-Spengler condensation between tryptamine or tryptophan derivatives and various substituted aldehydes or phenylglyoxals. These intermediates were then aromatized through oxidative dehydrogenation to yield the β -carboline core. Further modification at the C-7 carbonyl position using Wolff-Kishner reduction afforded 1-substituted β -carboline derivatives in moderate yields. The target daibucarboline A derivative was synthesized in four steps with an overall yield of 3.4%. Biological screening revealed that six of the synthesized compounds showed significant anti-inflammatory activity in a xanthine oxidase inhibitory assay, with inhibition rates of up to 63.17% at 100 μ g/mL. For anticancer evaluation, 55 β -carboline derivatives were virtually screened against five cancer cell lines (MCF7, MDA-MB-231, MCF10, HCT116, and HepG2). Five compounds displayed strong binding affinities toward targets A1b, A1f, A1j, A1m, and A2a, with docking scores ranging from -8.425 to -4.446 kcal/mol. These compounds also demonstrated favorable pharmacokinetic properties and lower predicted toxicity. All synthesized β -carboline intermediates and derivatives were structurally confirmed using NMR, FTIR, and GC-MS, supporting their potential as leads for next-generation anti-inflammatory and anticancer therapeutics.

Keywords: β -carbolines, daibucarboline A, Pictet-Spengler condensation, anti-inflammatory, anticancer

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ELUCIDATION OF THE ELECTROPHILIC POTENTIAL OF SOME BIOLOGICALLY ACTIVE MICHAEL RECEPTOR MOLECULES DERIVED FROM PLANTS

Basim H. Asghar^{a,*}, Nizar El Guesmi^{a,b,*}

^a Department of Chemistry, Faculty of Science, Umm Al-Qura University, Makkah, Saudi Arabia

^b Department of Chemistry, Faculty of Science, Monastir University, Monastir, Tunisia

*Corresponding author: bhasghar@uqu.edu.sa and naguesmi@uqu.edu.sa

Abstract

In recent decades, researchers have linked α,β -unsaturated carbonyl molecules to biological processes, revealing promising physiological properties of Michael acceptor molecules.¹ Many molecules under study are gaining interest due to their remarkable properties. Michael acceptor compounds also act as covalent inhibitors in COVID-19.¹ Compared to non-covalent inhibitors, covalent inhibitors exhibit higher affinity, more stable binding, and stronger effects. Due to its unsaturated aldehyde ketone structure, the Michael receptor molecule is classified as electrophilic.²⁻⁵ This means that it can form complexes with nucleophilic residues on proteins, which can either activate or block the protein pathway to play a physiological role. Therefore, the development of novel drugs or therapeutic candidates may be influenced by the understanding of the structure-function relationship of natural Michael acceptor molecules. The quantitative determination of nucleophilic and electrophilic reactivities is of great interest at the moment, especially in carbon-carbon and carbon-nitrogen bond formation processes.²⁻⁵ In this work we present the quantitative assessment of the reactions of the selected natural Michael acceptor molecules (Fig. 1) with various acceptor-substituted carbanions to determine the electrophilic reactivities of typical Michael acceptors. The kinetics of the reactions were studied photometrically in DMSO at 20°C. The reactions follow second-order kinetics, which was used to calculate the electrophilicity parameters E for compounds through Mayr's correlation $\log k (20^\circ\text{C}) = s(N + E)$.

Keywords: Michael acceptor molecules ; Electrophilicity ; Structure-reactivity relationships

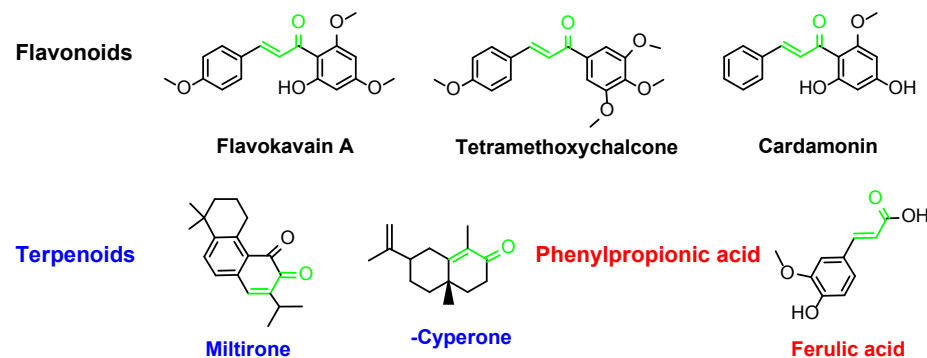


Fig. 1. Structure of natural Michael acceptor molecules (active sites are indicated in green).

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IN VITRO ANTIOXIDANT, ANTI-INFLAMMATORY, ANTI-CANCER AND IN SILICO MOLECULAR DOCKING STUDIES OF XANTHOSOMA SAGITTIFOLIUM (L) SCHOTT (YELLOW FLESH CULTIVAR)

Rachael Ekong^{a,b*}, Gloria Ndukwe^a, Ayodeji Oriola^b, Pallab kar^c, Godswill Fekarurhobo^a, Adebola Oyedeji^{b,c}

^a Department of Chemistry, Rivers State University, Port Harcourt, Rivers State, Nigeria

^b Department of Chemical and Physical Sciences, Walter Sisulu University, Mthatha, South Africa

^c African Medicinal Flora and Fauna Research Niche, Walter Sisulu University, Mthatha, South Africa

*Corresponding author: rachael.ekong2@ust.edu.ng

Abstract

Xanthosoma sagittifolium L (family Araceae) is a medicinal plant found in Africa, Southeast Asia, and America. Leaves of *X. sagittifolium* (XS) were investigated in this study for their chemical composition, and antioxidant, anti-inflammatory and anticancer activities. Phytocompounds present in XS were identified by liquid chromatography-mass spectrometry (LC-MS). *In vitro* antioxidant screening of XS ethanol extract was determined using 2,2-diphenyl-1-picrylhydrazyl (DPPH) and hydrogen peroxide (H₂O₂) assays. *In vitro* anti-inflammatory test was detected using the egg albumin denaturation (EAD) assay, while the 3-(4,5-dimethylthiazolyl-2)-2,5-diphenyltetrazolium bromide (MTT) cell viability assay was used to determine its anti-cancer potential. Lastly, the identified phytocompounds were molecularly docked against oxidative stress [NOX2 (7U8G)], inflammatory [NF-κβ (4DN5)], and cancer [mdm2 (3W69) and Bcl-xL (2YXJ)] proteins. LC-MS analysis of the extract revealed sixteen major compounds. The extract demonstrated notable DPPH and H₂O₂ radicals scavenging activities, with IC₅₀ values of 26.47±3.26 µg/mL and 11.94 ± 3.35 µg/mL respectively, and inhibition of EAD (IC₅₀ 12.67±1.67 µg/mL). The extract exhibited anticancer activity against U87 and U251 glioblastoma cells and MCF7 breast cancer cells with 72.6%, 52.2% and 74.3% viability respectively at a concentration of 100 µM. *In silico* studies revealed kaempferol-3-(2''-(*E*)-*p*-coumaroyl- α -L-arabinofuranoside)-7-rhamnoside, a flavonoid glycoside, as the most promising compound, demonstrating the highest binding energy scores of -9.60, -9.50 and -11.00 kcal/mol against NOX2, MDM2 and Bcl-xL proteins, respectively. Additionally, rutin, another flavonoid glycoside, exhibited a high binding energy score of -7.80 kcal/mol against NF-κβ (4DN5) protein. In conclusion, *X. sagittifolium* leaf extract showed considerable antioxidant, anti-inflammatory, and anticancer properties, which may be attributed to its putative compounds, especially the two flavonoid glycosides.

Keywords: *Xanthosoma sagittifolium*, Antioxidant, Anti-inflammatory, Anti-cancer

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DESIGN AND SYNTHESIS OF NOVEL α -MANGOSTIN'S ANALOGUES AS POTENTIAL NEUROPROTECTIVE AGENT

Shereen Lai Shi Min¹, Wei Meng Lim¹, Chee Wei Ang², Kooi Yeong Khaw¹

¹*School of Pharmacy, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, 47500 Selangor, Malaysia*

²*School of Science, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, 47500 Selangor, Malaysia*

Corresponding Author: khaw.kooiyeong@monash.edu

Abstract

Alzheimer's disease (AD) is one of the most common neurodegenerative disorders among the elderly. ADAM-10 is an enzyme that cleaves APP via α -secretase and generates a soluble amino-terminal fragment of APP called sAPP α , which exhibits neuroprotective properties¹. α -mangostin, a major xanthone from the pericarp of *Garcinia mangostana* possess neuroprotective properties. However, further research is needed to explore α -mangostin's potential for treating AD due to concerns over its toxicity². Hence, this study aimed to design and synthesise α -mangostin's analogues with reduced toxicity and improved neuroprotective properties. α -mangostin was extracted and isolated from the pericarp of *Garcinia mangostana*. It was used as a skeleton to synthesise five analogues through cyclisation on the targeted prenyl group and o-alkylation on the targeted hydroxyl group. MTT assay was then performed to determine the toxicity of the analogues towards SH-SH5Y cells, and western blot analysis was performed to assess their modulation potential against ADAM10. A total of five analogues (M1-M5) have been synthesized. MTT assay that was carried out on SH-SY5Y shows that the analogues have lower toxicity compared to α -mangostin, with 80% and above of cell viability even at high concentrations up to 20uM. Among the analogues, M2 has the least toxicity, with an IC₅₀ of 370uM, compared to α -mangostin, which has an IC₅₀ of 6.23uM. Western blot results show that M1 and M3 have an upregulation effect on ADAM10 among the analogues, with M1 being the most significant as it has a 1.5-fold upregulation effect on ADAM10.

Keywords: Alzheimer's diseases, α -mangostin, ADAM10, Neurodegenerative diseases

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SYNTHESIS AND BIOLOGICAL EVALUATION OF ALKALI METAL SALTS OF TRYPTANTHRIN-6-OXIME

Kovrizhina A.R. *, Khlebnikov A.I., Plotnikov E.V.

Tomsk Polytechnic University, 634050 Russia, Tomsk

*Corresponding author: anaskowry@gmail.com

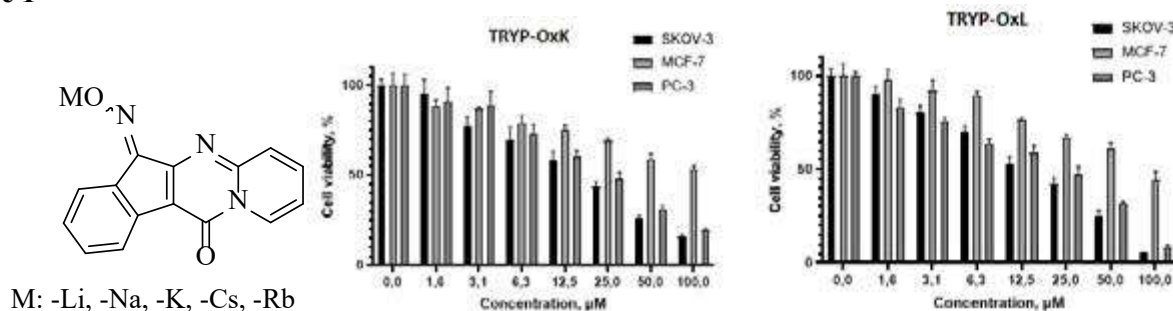
Abstract

Indolo[2,1-*b*]quinazolin-6,12-dione oxime (tryptanthrin-6-oxime, **Tryp-Ox**) exhibit a variety of chemical properties and pharmacological activities. Owing to ion-chelating properties, oximes can be ligands in various complexes formed by metal ions. As the complex formation can affect biological activity of oximes, we decided to obtain a series of alkali metal salts (oximates) containing the **Tryp-Ox** scaffold (Figure 1) and study their solubility and cytotoxicity. Previously we synthesized lithium and sodium salts of **Tryp-Ox** and established their high affinity for JNK1-3 ($K_d < 1 \mu\text{M}$) and potent inhibition of LPS-induced nuclear NF- κ B/AP-1 activation and IL-6 production in human monocytic cells [1]. The c-Jun N-terminal kinase (JNK) pathway is a dual-functional oncogenic signaling that exerts both anti- and pro-tumor activities [2,3]. In this research we focused on evaluation the antitumor activity of oximates.

The ^1H NMR spectra of the synthesized oximates do not show a singlet of the oxime proton. In addition, the salts are characterized by high melting points ($>300^\circ\text{C}$). The **Tryp-Ox** salts have higher solubility in water than the starting tryptanthrin-6-oxime, which in turn indicates greater bioavailability. It has been preliminarily established that at concentrations of $25 \mu\text{M}$, $12.5 \mu\text{M}$ and $6.25 \mu\text{M}$ the studied samples have a dose-dependent cytostatic effect on prostate cancer cells of the PC-3 line, ovarian cancer – SKOV-3, breast cancer – MCF-7, since inhibition of cell growth without cell death is observed. The most pronounced inhibition of tumor cell growth was observed for compounds potassium and lithium salts (Figure1). Morphologically, the cells retained their shape, and the number of dead cells corresponded to the control group. For all compounds, viability parameters were calculated and inhibitory concentrations IC_{50} were established.

Keywords: alkali salts, tryptanthrin-6-oxime, solubility, cytotoxicity

Figure 1



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PIPERIDINE-AROMATIC AMINE HYBRIDS IN IMMUNOTHERAPY APPROACHES

Malmakova A.E.^{a,b,*}, Yu V.K.^{a,b}, Baktybayeva L.K.^c

^a Kazakh-British Technical University, Almaty, Kazakhstan.

^b Bekturov Institute of Chemical Sciences, Almaty, Kazakhstan.

^c Al-Farabi Kazakh National University, Almaty, Kazakhstan.

*Corresponding author: malmakova@mail.ru

Abstract

Piperidine-aromatic amine hybrids' characteristics are essential to their function in drug development, highlighting their significance in medicinal chemistry. Although many studies indicate the potential role of piperidine-aromatic amine hybrids in immunoregulation, the mechanism of their action and their effective role in various aspects of immune function require additional study.

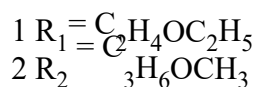
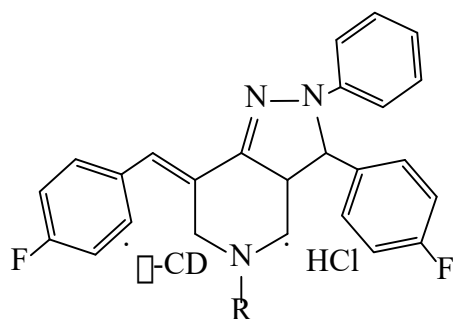
Throughout our study (3,4), series of piperidine-amine hybrids were described, which had high myelostimulating activity with piperazine and morpholine substituents at the nitrogen atoms of the bicyclic piperidine ring. Activity was lost when pyridine was used in place of the morpholine or piperazine ring in bicyclic piperidine. However, after acylation with O-benzoyl chloride N-pyridine substituted 3,7-diazabicyclo[3.3.1]nonan-9-one stimulated both erythro- and leukopoiesis while its N-piperazine analog stimulated only leukopoiesis. 2 β -cyclodextrin complexes of pyrazolines has been studied for myelostimulating activity. All blood data were compared with indicators of methyluracil.

Compound 1 greatly accelerated the division of lymphocyte cells and the relative lymphocyte index reached the value of $(93.99 \pm 1.9) \%$, the relative neutrophil and granulocyte-monocyte indices were critically low and amounted to $(2.72 \pm 0.1) \%$ and $(3.44 \pm 0.1) \%$ respectively. Administration group likewise had a successful restoration of platelet levels. Compared to the control group's value of $228.5 \pm 6.5 \cdot 10^9/L$ of blood, the total platelet index achieved a value of $548.0 \pm 32.41 \cdot 10^9/L$ of blood.

Compound 2 efficiently induced leukocyte cell growth. The total leukocyte index was 2.11 times higher than the placebo group's blood $(3.75 \pm 0.7) \cdot 10^9/L$ and marginally higher than the control group's $(7.92 \pm 0.5) \cdot 10^9/L$ blood. The experimental group had a total platelet count of $(477.50 \pm 21.05) \cdot 10^9/L$ of blood, which was 2.08 times greater than the control group.

Compound 2 stimulated leukopoiesis at the level compared to methyluracil. It was distinguished by a pronounced stimulation of the lymphocyte pool with a pathological critical decrease in granulocytic-monocyte indicators.

Keywords: Piperidine-aromatic amine hybrid, 3,7-diazabicyclo [3.3.1] nonan-9-one, myelostimulating activity



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3. *The research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP22685628).*

PALLADIUM-MEDIATED SITE-SELECTIVE C–H BOND ACTIVATION AND ARYLATION OF 9(10*H*)-ACRIDINONE AND MECHANISTIC INVESTIGATION: STOICHIOMETRIC AND CATALYTIC APPROACHES

Jean-Ho Chu^{a,*}, Jin Lee^a, Guan-Wei Liao^a, Lin-En Zeng^a, Chien-Wen Lin^a, Ching-Hung Cheng^a, Wen-Chieh Lin^a, Li-Ching Shen^b, Guo-Feng Chen^c, Rong Chang^d, Andrew C.-H. Sue^d

^aDepartment of Applied Science, National Taitung University, Taitung 95092, Taiwan R.O.C.

^bDepartment of Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu 300093, Taiwan, R.O.C.

^cDepartment of Chemistry, National Chung Hsing University, Taichung 402202, Taiwan, R.O.C.

^dCollege of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

*Corresponding author: j_hchu@nttu.edu.tw

Abstract

9(10*H*)-Acridinones¹ are significant classes of organic compounds that have garnered considerable attention in medicinal chemistry due to their potent bioactivities. Additionally, 9(10*H*)-acridinone derivatives often exhibit good fluorescence properties, making them suitable for use in chemical sensors and biological imaging. Therefore, developing facile and efficient methodologies for its structural derivatization is becoming crucial. In this work, palladium-mediated site-selective C–H bond activations of 9(10*H*)-acridinone, resulting in the formation of 4- and 1-arylated 9(10*H*)-acridinones, are presented through the use of both stoichiometric and catalytic experiments. In the stoichiometric reactions, two distinct classes of acridinone palladacycles are generated via C (4)–H and C (1)–H bond activations, with the pyridine and ketone groups serving as the directing group, respectively. The constitutional conformation and thermal stability of these palladacycles were elucidated through both X-ray crystallography and NMR spectroscopy. Additionally, an investigation was conducted into the interconversion of C (4 and 1)–H bond-activated palladacycles in trifluoroacetic acid and acetic acid. During the course of C (1)–H bond arylation, a serendipitous discovery led to the isolation of a chromeno [4,3,2-*kl*] acridinone compound as a byproduct, showcasing good fluorescence properties. Controlled experiments, kinetic isotope effect study, key palladacycles, and the formation of corresponding products support the proposed mechanisms for these presented reactions. Finally, we believe that the presented study will benefit chemists in gaining insights into mechanisms for Pd-mediated C–H bond activation and functionalization/transformation.

Keywords: C–H Bond Activation, 9(10*H*)-Acridinone, Palladium, Arylation



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SYNTHESIS OF COUMARINOLIGNOID SAPIUMIN C ANALOGS UTILIZING RHODIUM CATALYZED ARYLATION

Irene Jeongin Kim^{1*}, Patrick Pan², Lisa I. Pilkington^{1,3} and David Barker^{1,4*}

¹ School of Chemical Sciences, University of Auckland, 23 Symonds St, Auckland, New Zealand

² School of Pharmacy, Faculty of Medical and Health sciences, University of Auckland, Auckland 1142, New Zealand

³ Te Pūnaha Matatini, Auckland 1010, New Zealand

⁴ MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

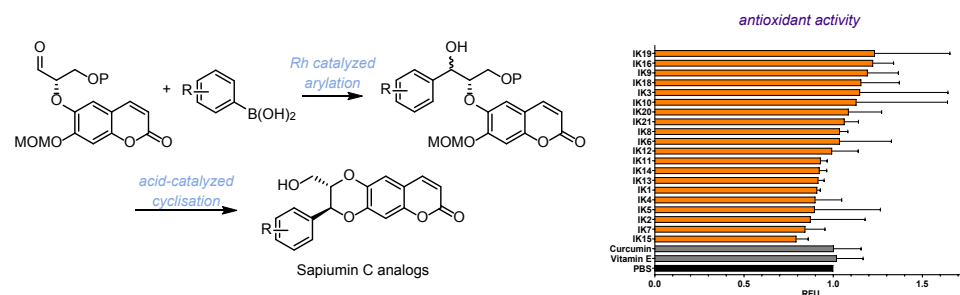
*Corresponding author: d.barker@auckland.ac.nz , ikim110@aucklanduni.ac.nz

Abstract

Coumarinolignoids (CLs) are a class of natural benzodioxane products that exhibit a wide range of interesting biological activities, including hepatoprotective, antitumor, anti-inflammatory, and antioxidant activity and among others.^{1–3} Previously, in our research, an asymmetrical total synthesis had been previously developed to synthesize natural CLs (-) and (+)-sapiumin C, (-)-moluccanin and (-)-hemidesmine and other benzodioxanes such as (-) amovillosumin A and C.^{3,4} A key reaction in the synthesis is a Rh-catalyzed arylation of complex aliphatic aldehydes which was further investigated to broaden the scope using a diverse range of arylboronic acids. The reaction is neither time, temperature nor moisture sensitive and is much less hazardous and greener than the conventional arylations such as Grignard and organolithiation additions.^{4,5} Subsequently, the alcohol products were then cyclized to synthesize a library of chiral analogs of sapiumin C and other benzodioxane lignan based compounds on which antioxidant testing was conducted. The preliminary testing showed some compounds had good antioxidant activity, displaying stronger antioxidant activity than the positive control of curcumin and Vitamin E at the concentration of 1 μM for 3 hours.

Keywords: Lignan, Coumarinolignoid, Rhodium catalysis, organometallic arylation additions, antioxidant activity

Graphic / Image



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IRIDIUM-CATALYZED DECARBONYLATIVE ANNULATION OF BENZOIC PIVALIC ANHYDRIDES WITH ALKYNES

Takanori Matsuda^{a*}, Koichiro Yamada^a, Yixuan Lin^a, Yuki, Ito^a, Hirotugu Suzuki^b

^aDepartment of Applied Chemistry, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan

^bTenure-Track Program for Innovative Research, University of Fukui, 3-9-1 Bunkyo, Fukui-shi, Fukui 910-8507, Japan

*Corresponding author: mtd@rs.tus.ac.jp

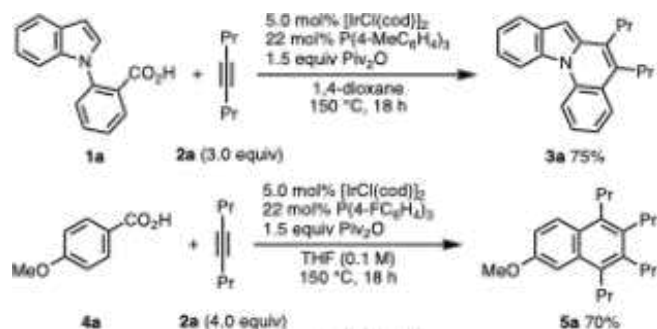
Abstract

The synthesis of polycyclic aromatic compounds is a critical area of research due to their diverse applications as key intermediates in organic semiconductors and luminescent materials. Among the various synthetic strategies, transition-metal-catalyzed benzannulation stands out as one of the most straightforward and efficient methods. Traditionally, these reactions have often relied on the use of oxidants, highlighting the importance of exploring redox-neutral conditions for benzannulation.

In this study, we present two types of annulation reactions with alkynes, leading to the synthesis of substituted indolo[1,2-*a*]quinolines and naphthalenes via the decarbonylation of benzoic pivalic anhydrides. These transformations are catalyzed by iridium(I) complexes under oxidant-free conditions. This method has been successfully applied to synthesize a diverse array of polycyclic aromatic compounds, demonstrating its broad versatility and practical applicability.

When 2-(1*H*-indol-1-yl)benzoic acids (**1**) and oct-4-yne (**2a**, 3.0 equiv) were heated in 1,4-dioxane at 150 °C for 18 h in the presence of [IrCl(cod)]₂ (5.0 mol%) and P(4-MeC₆H₄)₃ (22 mol%), the desired annulation product, indolo[1,2-*a*]quinoline **3a**, was obtained in a 75% isolated yield.¹ Similarly, the reaction of 4-methoxybenzoic acid (**4a**) with **2a** and pivalic anhydride under analogous conditions afforded 6-methoxy-1,2,3,4-tetrapropynaphthalene (**5a**) in a 70% isolated yield. The scope and limitations will be also presented.

Keywords: iridium; annulation; aromatic compounds; anhydrides; decarbonylation



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NOVEL ANTIPARKINSONIAN AGENTS BASED ON PROTTREMIC

Nikolai Li-Zhulanov*, Alexandra Podturkina, Anastasia Filippova, Alla Pavlova, Konstantin Volcho, Tatyana Tolstikova, Nariman Salakhutdinov

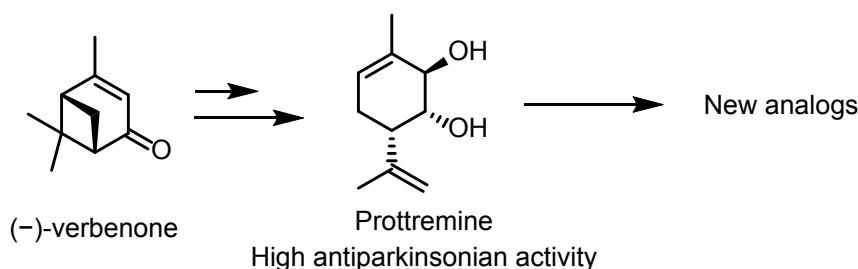
Novosibirsk Institute of Organic Chemistry of SB RAS, Novosibirsk, 630090, Lavrentiev av., 9, Russia

*Corresponding author: lizhulan@nioch.nsc.ru

Abstract

Parkinson's disease (PD) is a progressive neurodegenerative disorder primarily characterized by movement dysfunction. It has been demonstrated that Prottremine ((1*R*,2*R*,6*S*)-3-methyl-6-(prop-1-en-2-yl)cyclohex-3-ene-1,2-diol) exhibits antiparkinsonian activity *in vivo* across various animal models of PD^{1,2} and has successfully completed the first phase of clinical trials³. Modification of Prottremine allows obtaining more active compounds against PD⁴. In addition, it can be used to obtain polycyclic heterocycles with diverse biological activity⁵. The present work aimed at creating new derivatives of Prottremine. Antiparkinsonian tests demonstrated that some of new derivatives of Prottremine showed high antiparkinsonian activity in the MPTP model in mice.

Keywords: drug design; medicinal chemistry; monoterpenoids; natural products; Parkinson's disease



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ISOLATION OF CARBAZOLE ALKALOIDS FROM *MURRAYA KOENIGII* LEAVES

Viven Ting^a, Hui-Yin Tan^b, Siow-Ping Tan^{a,*}

^aDepartment of Physical Science, Tunku Abdul Rahman University of Management and Technology,
53300 Kuala Lumpur, Malaysia.

^bFaculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology,
53300 Kuala Lumpur, Malaysia.

*Corresponding author: tansp@taru.edu.my

Abstract

Murraya koenigii comes from the family Rutaceae and is commonly known as curry leaf. It is widely grown across Southeast Asia, mainly in India and Sri Lanka. *Murraya koenigii* is known for its carbazole alkaloids which interacts intricately to produce pharmacodynamic effects. In this study, carbazole alkaloids will be isolated and characterized. The leaves of *Murraya koenigii* was macerated with hexane, dichloromethane and methanol to produce three crude extracts. From the hexane crude, eight fractions were eluted via column chromatography. Two compounds had been successfully isolated via preparative thin layer chromatography with a solvent system of hexane:DCM (3:2). Both compounds were characterized by NMR (1D and 2D spectroscopy) and FTIR. They are successfully identified as murrayazolinol **1** and mahanimbine **2**, respectively. When tested individually on thin layer chromatography, murrayazolinol with a solvent system of hexane:DCM (1:1) had an R_f value of 0.62 while mahanimbine with a solvent system of hexane:DCM (2:3) had an R_f value of 0.69. Mahanimbine and girinimbine are two compounds with promising biological activities, therefore the next focus on this project is to isolate girinimbine and test on both of their anti-inflammatory properties.

Keywords: Carbazole alkaloids, *Murraya koenigii*, Rutaceae, Mahanimbine, Murrayazolinol

PANCREATIC LIPASE INHIBITORY EFFECTS OF *MURRAYA KOENIGII* ROOT EXTRACTS

Wai Ting Chong^a, Sook Yee Liew^{b,c}, Siow Ping Tan^{a,*}

^a Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, 53300 Kuala Lumpur, Malaysia.

^b Chemistry Division, Centre for Foundation Studies in Science, Universiti Malaya, Kuala Lumpur, Malaysia.

^c Centre for Natural Products Research and Drug Discovery (CENAR), Universiti Malaya, Kuala Lumpur, Malaysia.

Abstract

Obesity is a growing health problem in many countries including Malaysia. *Murraya koenigii* also knowns as curry tree, is a traditional herbal remedy from the family of Rutaceae for its wide range of traditional uses and pharmacological properties. It was used to treat numerous diseases such as diarrhoea, flatulence, fever, renal pains, insect bite and so on due to the presence of carbazole alkaloids. While previous studies have shown its effectiveness as an anti-obesity agent in live animals through in vivo testing, the phytochemical components of this plant responsible for this effect remain relatively unexplored. The dried roots of *M. koenigii* were extracted sequentially using hexane, dichloromethane, and methanol by maceration method. These extracts were then evaluated of its pancreatic lipase inhibitory activity through in vitro assay. Among the crude extracts, methanolic extract exhibited the highest inhibitory activity of 75.30%, followed by DCM extract (48.03%) and hexane extract (37.08%) at concentration of 10 mg/mL, respectively. The methanolic root extract of *M. koenigii* demonstrated significant activity inhibiting the pancreatic lipase with an IC₅₀ value of 3.1605 µg/mL. Therefore, this study is conducive to further investigation the phytochemical composition, pharmacological properties, and toxicity of *Murraya koenigii*, and provides a foundation for future research in phytomedicine.

Keywords: *Murraya koenigii*, antiobesity, maceration, pancreatic lipase inhibitory activity, Rutaceae.

STRUCTURE-ACTIVITY RELATIONSHIP OF CARBAZOLE ALKALOIDS ISOLATED FROM *MURRAYA KOENIGII* AGAINST CANCER CELL LINES

Ying Xin Chew^a, Mohd Azlan Nafiah^b Siow Ping Tan^{a*}

^a*Department of Physical Sciences, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Malaysia.*

^b*Department of Chemistry, Faculty of Science and Mathematics, University Pendidikan Sultan Idris, Tanjong Malim, Perak, Malaysia.*

^{*}*Corresponding author: tansp@tarc.edu.my*

Abstract

Carbazole alkaloids, a class of bioactive natural compounds, have gained attention for their potential anticancer properties. Hence, to understand the relationship between the structural features of carbazole alkaloids, and their potency in cytotoxic activities, the present study, the structure-activity relationship (SAR) analysis of several carbazole alkaloids (**Mk1-Mk30**) isolated from *Murraya koenigii* was performed. This analysis was performed by investigating their cytotoxic effects against human promyelocytic leukemia (HL-60) and cervical cancer cell lines (HeLa) cancer cell lines. The results indicate that substitutions on the tricyclic carbazole nucleus had no clear correlation with cytotoxic potency. **Mk2** exhibited the highest potency due to ortho- and para-positioned electron-donating groups, while other substituents resulted in reduced activity. Moreover, **Mk10** and **Mk11** showed enhanced cytotoxic activity attributed to the presence of quinone ring system. In contrast, cyclic monoterpenoid pyrano[3,2-a]carbazole alkaloids (**Mk23-Mk25**) demonstrated generally weak cytotoxicity, except for **Mk26**, which showed strong activity due to the presence of additional electron-donating group. Furthermore, binary carbazole alkaloids (**Mk27-Mk30**) exhibited weak activity, suggesting that the symmetrical dimerization leads to a decrease in cytotoxic potential. Overall, the SAR investigation has revealed that the presence of electron-donating and electron-withdrawing groups have great impact on the cytotoxic activities against HL-60 and HeLa cancer cells, whereas the position of the substituents in the carbazole nucleus play an important role in the activities. The important structural features of carbazole-based anticancer agents were identified.

Keywords: SAR, Carbazole alkaloids, *Murraya koenigii*, HL-60, HeLa cancer cell lines.

MECHANOCHEMICAL SYNTHESIS OF α,β -DIBROMOKETONES USING PYRIDINIUM TRIBROMIDE

Wei-Jin Chang^a, Sook-Yee Liew^{b, c}, Thomas Kurz^d, Siow-Ping Tan^{a, *}

^aDepartment of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Malaysia.

^bChemistry Division, Centre for Foundation Studies in Science, Universiti Malaya, Kuala Lumpur, Malaysia.

^cCentre for Natural Products Research and Drug Discovery (CENAR), Universiti Malaya, Kuala Lumpur, Malaysia.

^dInstitute of Pharmaceutical and Medicinal Chemistry, Heinrich-Heine Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany.

*Corresponding author: tansp@tarc.edu.my

Abstract

α,β -dibromo compounds are important intermediates in the synthesis of epoxides or 1,2-diols, and for converting the α -position of the ketone into an electrophilic atom reactive to substitution to construct larger molecules. α,β -dibromo compounds can be synthesized from alkenes through bromination under different reaction conditions, such as bromide/bromate coupling system ¹, *N*-bromosuccinimide/lithium bromide system ², tetrabutylammonium bromide ³ and ceric ammonium nitrate/ammonium bromide ⁴. Chemical reactions possess activation energy barriers which must be overcome in order to proceed. Traditionally, the energy is provided by conventional heating of the reaction mixtures using heating plates or oil baths. However, modern methods of providing energy to the reaction mixture have progressed, such as microwave irradiation, sonication and mechanical grinding. These methods enable reactions to be conducted at lower temperatures, even possibly under ambient temperatures, which saves energy and reduces the formation of by-products. Mechanical grinding can be conducted in a simple mortar and pestle set up, or in more complicated settings such as ball-milling. The objectives of this study is to conduct bromination of α,β -unsaturated ketones using the brominating agent pyridinium tribromide under mechanochemical conditions. Methodologically, the α,β -unsaturated ketones **2a** and **2b** prepared from aldol condensations were mixed with pyridinium bromide and grinded followed by simple aqueous work-up, filtration and drying of the precipitated product, which were characterized using ¹H and ¹³C Nuclear Magnetic Resonance (NMR). The α,β -dibromoketone compounds **2a** and **2b** were obtained in good to excellent yields of 75% and 95%. The ¹H NMR doublets at 6.8/5.4 ppm 6.0/4.9 ppm support the formation of the α,β -dibromo adduct. In conclusion, α,β -dibromoketones were synthesized through mechanochemical-assisted bromination by pyridinium tribromide.

Keywords: α,β -dibromoketone, bromination, pyridinium tribromide, mechanochemical.

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MECHANISM OF ACTION AND CATALYTIC EFFICIENCY OF DICYANOPYRAZINE PHOTOREDOX CATALYST

Miroslav Ludwig^{a*}, Zuzana Burešová^a, Monika Grygarová^a, Pavlína Perglová^a, Filip Bureš^a

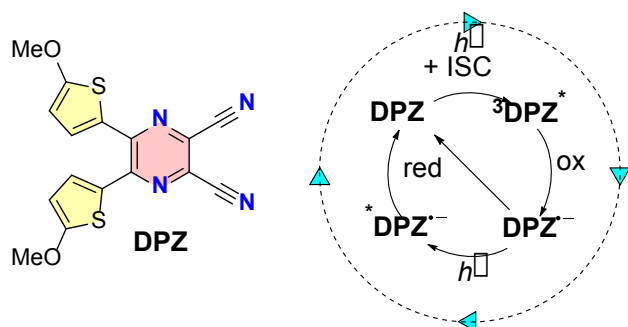
^a*Institute of Organic Chemistry and Technology, Faculty of Chemical Technology, University of Pardubice, Czech Republic, Studentská 573, Pardubice 53210, Czech Republic.*

**Corresponding author: mirosla.ludwig@upce.cz*

Abstract

Visible light is considered a valuable and eco-friendly tool for performing radical transformations. In photoredox catalysis, the energy of light is combined with a light-absorbing molecule (photoredox catalyst) to achieve its excited state (more potent redox agent) and to enable radical reactions on unprecedented substrates with high selectivity under mild reaction conditions.¹ Historically, organic catalysts such as xanthene dyes, acridinium salts, flavins, and (di)ciano(hetero)arenes² have demonstrated remarkable activity in numerous photoredox transformations. In 2014, X-shaped dicyanopyrazine (DPZ)³ photocatalyst has been synthesized in our working group and subsequently its multigram synthesis⁴ and potential applications have been explored.⁵ The recent photophysical and theoretical study disclosed DPZ's fundamental mechanism of action and its catalytic efficiency.⁶ Hence, this contribution will discuss the fundamental photophysical properties, including optical properties, electrochemistry, ground and excited state reduction potentials, and their correlation to the DPZ's catalytic activity in selected photoredox reactions such as cross-coupling, deuteration of aldehydes, and annulation.

Keywords: dicyanopyrazine, photoredox catalysis, mechanism



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COPPER-CATALYSED SYNTHESIS OF PROPARGYL ALCOHOL AND DERIVATIVES FROM ACETYLENE AND OTHER TERMINAL ALKYNES

Leo Saputra,^a Nikolai A. Sitte,^a Francesca Ghiringhelli,^a Grigory A. Shevchenko,^b Frank Rominger,^c Stephen K. Hashmi,^{a,c} Thomas Schaub,^b Jaroslaw Mormul^{a,b,*}

^aCatalysis Research Laboratory (CaRLa), Im Neuenheimer Feld 271, D-69120 Heidelberg, Germany

^bBASF SE, Chemical Synthesis Research, Carl-Bosch-Straße 38, D-67056 Ludwigshafen, German

^cInstitute of Organic Chemistry, Heidelberg University, Im Neuenheimer Feld 270, D-69120 Heidelberg, Germany

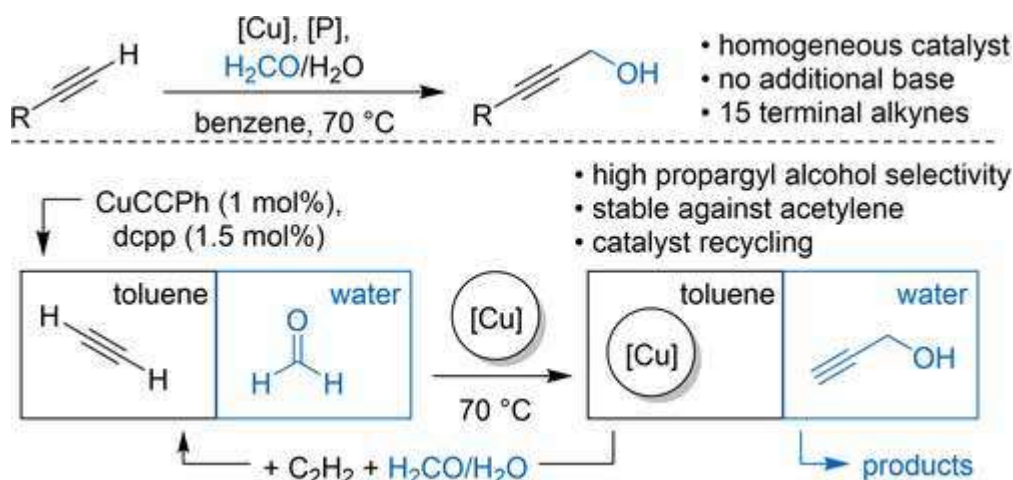
*Corresponding author: jaroslaw.mormul@basf.com

Abstract

A copper(I)/phosphine system that homogeneously catalyses the alkynylation of formaldehyde with acetylene or terminal alkynes is reported.¹ Using acetylene at atmospheric pressure, the catalyst consisting of copper(I) phenylacetylide (<1 mol% loading to the substrate) and a trialkyl bisphosphine ligand shows a high selectivity towards the formation of propargyl alcohol rather than 1,4-butyne-1,3-diol, which is not reported for common heterogeneous copper acetylide catalysts. The biphasic water/toluene reaction mixture allows the separation of targeted products with the aqueous layer and catalyst recycling via the organic layer.

Keywords: biphasic catalysis, copper, phosphine ligands, alkynes, alcohols

Graphic / Image (Optional)



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SYNTHESIS OF 2,4,5-TRISUBSTITUTED OXAZOLES FROM COPPER-MEDIATED BENZYLIC sp^3 C–H AEROBIC OXIDATIVE ANNULATION OF KETONES AND AMINES VIA A CASCADE REACTION

Mncedisi Mazibuko^a, Vineet Jeena^{a*}

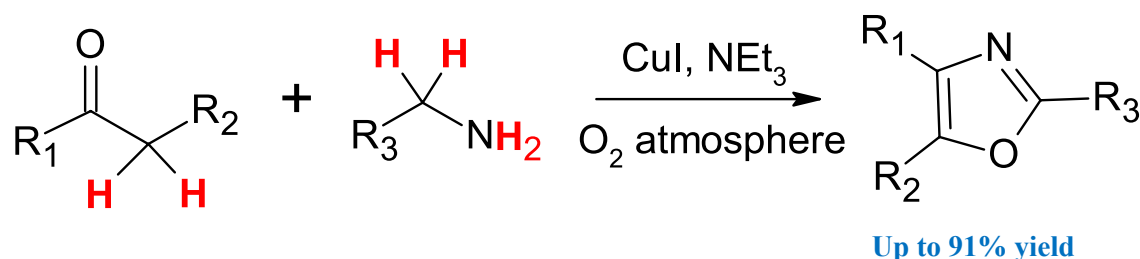
^a School of Chemistry and Physics, University of KwaZulu-Natal, Scottsville, Pietermaritzburg 3209, South Africa.

*Corresponding author: jeenav1@ukzn.ac.za

Abstract

2,4,5-Trisubstituted oxazoles are of vital importance in medicinal chemistry as they form the backbone of many commercially available drugs [1]. A common approach to these fascinating compounds is the reaction between an α -diketone and benzylamine under various reaction conditions [2]. We have expanded this synthetic methodology by commencing from an α -methylene ketone, rather than the traditional diketone, using C–H oxidation as a key step [3]. Using a copper/ NEt_3 system, a series of diverse trisubstituted oxazoles were prepared in good to excellent yields under mild reaction conditions (**Scheme 1**) [3]. Preliminary mechanistic studies suggested that the reaction proceeds by an anionic-type mechanism via the formation of a keto-imine intermediate [3]. The synthetic methodology is attractive due to the removal of six hydrogen atoms, functionalization of one sp^2 carbon and two sp^3 carbons as well as the formation of C–O and C–N bonds.

Keywords: Copper, Oxazoles, Oxidative



Scheme 1

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RYLENEDIIMIDE-TRIAZINYL RADICALS: INITIAL STUDY

Georgia A. Zissimou^{a,*}, Christos P. Constantinides^b, Daniel B. Lawson^b, Panayiotis A. Koutentis^a

^aDepartment of Chemistry, University of Cyprus, P.O. Box 20537, 1678 Nicosia, Cyprus

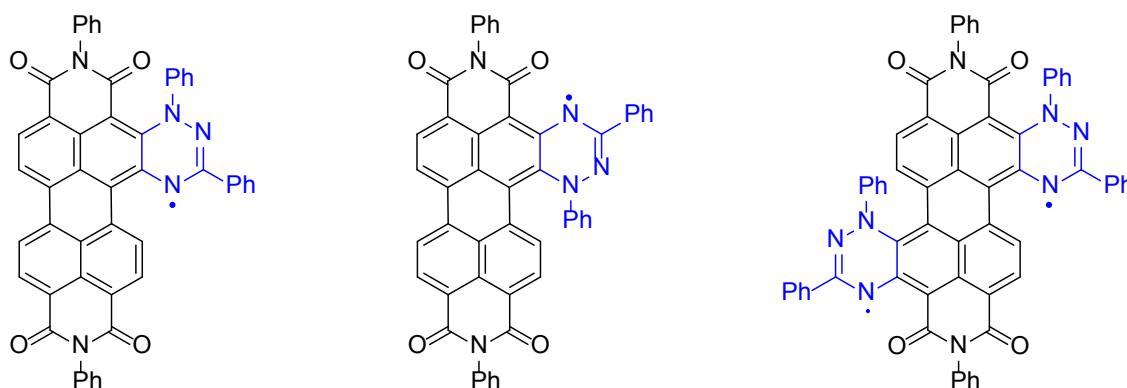
^bDepartment of Natural Sciences, University of Michigan – Dearborn, 4901 Evergreen Rd, Dearborn, MI 48128, United States

*Corresponding author: gzissi01@ucy.ac.cy

Abstract

Organic spintronic devices necessitate stable, high-spin molecules that retain their magnetic properties under ambient conditions and device operation¹. One promising class of stable high-spin systems are the triazinyl radicals²⁻⁵ which can be further tuned by incorporating extended π -conjugated systems, such as rylenediimides⁶. In this initial study we investigate rylenediimide (RI)-fused 1,2,4-benzotriazin-4-yls (Blatter radicals) as promising candidates. Density Functional Theory (DFT) calculations demonstrate that [e]-ring fusion of the triazinyl moiety onto the RI core enhances molecular planarity and rigidity, facilitating extensive spin delocalization across the amidrazone unit and the π -conjugated backbone. Our calculations demonstrate that this delocalization stabilizes the radical conjugates, resulting in low singlet-triplet energy gaps ($\Delta E_{ST} < -2$ kcal/mol). These findings suggest that RI-fused Blatter radicals exhibit robust paramagnetism and offer a platform for tuning magnetic properties, making them attractive building blocks for the development of advanced organic spintronic devices.

Keywords: organic radicals, magnetism, spintronics



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LADDER-TYPE FUSED BENZODITHIOPHENE-BASED NON-FULLERENE ACCEPTORS FOR HIGH-EFFICIENCY ORGANIC SOLAR CELLS

Longyun Shi, Ning Yang, Do-Hoon Hwang*

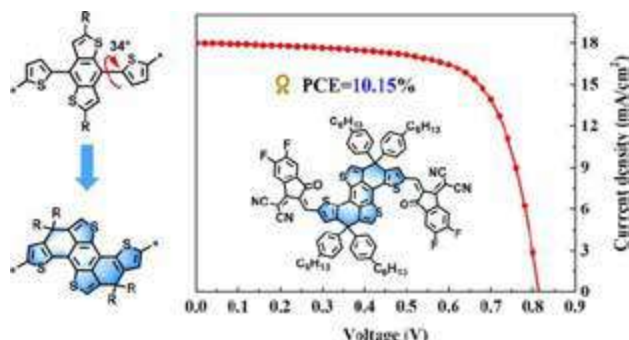
Pusan National University

*Corresponding author: dohoonhwang@pusan.ac.kr

Abstract

Ladder-type fused aromatic systems serve as essential core structures in small-molecule acceptors for organic solar cells (OSCs). In this study, we investigate a novel ladder-type donor building block based on the benzo[1,2-b:4,5-b']dithiophene (BDT) unit. In this structure, a seven-ring core, denoted as f-DTBDT, is formed by fusing the 3,7 positions of the BDT thiophene rings and the 3' position of the thiophene rings of the vertically aligned BDT unit. The fusion at the 4,8 positions of BDT further constrains the entire aromatic system into a coplanar conformation, enhancing structural rigidity and electronic delocalization. The newly designed f-DTBDT was employed as a core donor building block and conjugated with three electron-withdrawing acceptor units—2-(3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (2HIC), 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (2FIC), and 2-(5,6-dichloro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (2ClIC)—to construct acceptor-donor-acceptor (A-D-A) type acceptor materials for OSCs. Characterization of the synthesized A-D-A acceptors, DTBDT-IC, DTBDT-4F, and DTBDT-4Cl, revealed strong absorption in the visible–near-infrared (vis–NIR) region, attributed to the intramolecular charge transfer interaction between the f-DTBDT core and the terminal acceptor groups.¹

Keywords: ladder-type building block, carbon bridge, vertical benzodithiophene, fused aromatic rings



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SYNTHETIC STRATEGIES TO BIOACTIVE β -CARBOLINES

Ahmad Saifuddin Mohamad Arshad^{a,*}, Nur Aziah Hanapi^a, Mohd Nizam Mordi^a

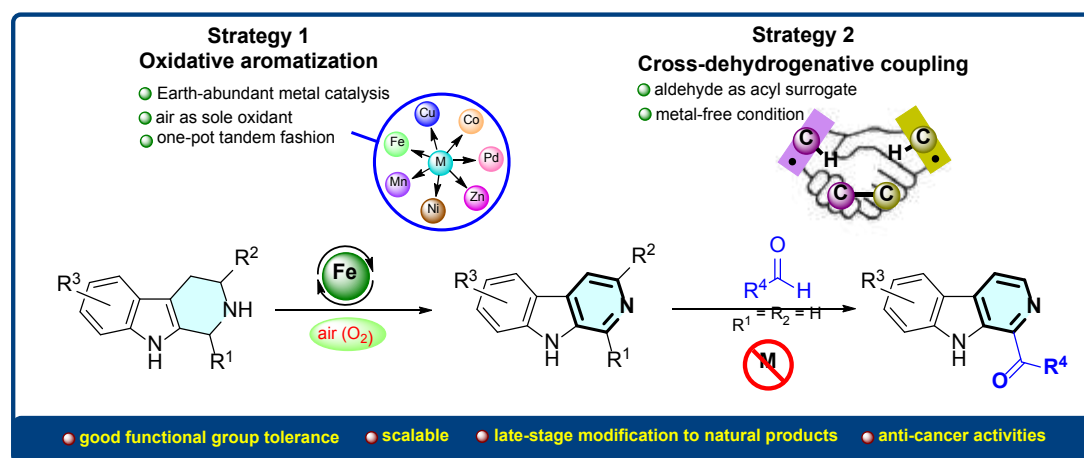
^aCentre for Drug Research, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

*Corresponding author: saifudin_pudin@yahoo.com

Abstract

β -Carbolines, a distinguished family of indole alkaloids, occupy a prominent position in medicinal chemistry, with their diverse bioactivities rendering them invaluable scaffolds for drug discovery, particularly in the fight against cancer, infections, and central nervous system (CNS) disorders. The unique structural features of these tricyclic compounds enable them to engage with a wide array of biological targets, making them highly attractive candidates for therapeutic development. It is therefore entirely understandable that β -carbolines are often a major focus in organic and medicinal chemistry. This work explores into the synthetic strategies employed to access bioactive β -carbolines, focusing on addressing key challenges that have historically impeded their efficient synthesis and development. First, we developed greener aerobic transition-metal catalytic system for tetrahydro- β -carboline oxidative aromatization, replacing traditional stoichiometric oxidants.¹ While this method is versatile for introducing various aromatic substituents, incorporating acyl groups posed a challenge due to the limited availability of α -oxoaldehyde. Furthermore, inherent selectivity issues associated with existing synthetic procedures have long plagued β -carboline synthesis, often resulting in low yields and limiting the practicality of these methods. To overcome this, we introduced a Minisci-type cross-dehydrogenative coupling reaction, enabling the efficient acylation of the β -carboline core.² Finally, we evaluate the cytotoxic activity of a library of synthesized β -carboline derivatives against cancer cell lines, establishing structure-activity relationships through systematic structural modifications. These findings contribute to the development of more sustainable and efficient synthetic strategies and provide insights into the design of β -carboline-based therapeutics.

Keywords: β -carbolines, oxidative aromatization, Minisci reaction, cross-dehydrogenative coupling



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PHYTOCHEMICAL AND PHARMACOLOGICAL INVESTIGATION OF MANGROVE PLANT SPECIES FROM SINE-SALOUM (SENEGAL) USING ETHNOPHARMACOLOGICAL APPROACH AND MOLECULAR NETWORKING

C. Gaye^{a,b*}, D. Fall^b, Y. Tine^b, E. Garayev^a, A. Bousquet-Mélou^a, B. Baghdikian^a

^a Aix Marseille Univ, Avignon Univ, CNRS, IRD, IMBE, Marseille, France

^b Cheikh Anta Diop University, Dakar, Senegal

*Corresponding author: djibril.fall@ucad.edu.sn

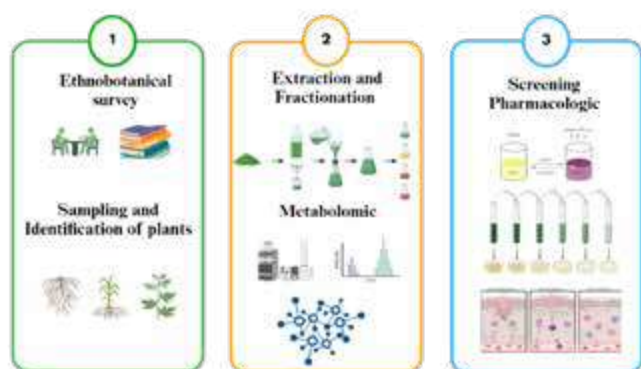
Abstract

Mangroves are unique coastal forests found at the land-sea interface in tropical and subtropical regions (Alongi, 2002). These ecosystems, primarily composed of mangrove trees, thrive under extreme environmental conditions such as low oxygen levels due to tidal flooding, high salinity, strong winds, and elevated temperatures. Their ability to survive in such harsh conditions is attributed to morphological and physiological adaptations, including the production of specialized secondary metabolites. These bioactive compounds, such as alkaloids, polyphenols, and terpenes, play key roles in ecosystem function and have significant potential for medicinal applications.

This study examines the pharmacological properties and phytochemical composition of six mangrove species from the Sine-Saloum region of Senegal, using an ethnopharmacological approach. The main objective is to deepen the understanding of these plant species by analyzing their chemical composition, validating their pharmacological activities, and characterizing the metabolites responsible for these properties.

A combination of advanced computational metabolomics and mass spectrometry-based molecular networking approaches was used to profile the phytochemical diversity of these species. Molecular networks facilitate structural dereplication and enable the analysis of large datasets, thus providing a comprehensive overview of the chemical composition of plants. This metabolomic study aims to establish a detailed chemical profile of mangrove species, contributing to the valorization of their bioactive compounds and their potential therapeutic applications.

Keywords: Mangroves, Senegal, ethnopharmacology, phytochemistry, metabolomics, molecular networking.



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LIGAND-FREE CuCl-CATALYZED N-ARYLATION OF 1,2,4-TRIAZOLE WITH ARYL BROMIDES

Yong-Chua Teo^{a,*}, WeiZhi Ang^a, Chloe Kah-Yee Low^a,

^a National Institute of Education, Nanyang Technological University

*Corresponding author: yongchua.teo@nie.edu.sg

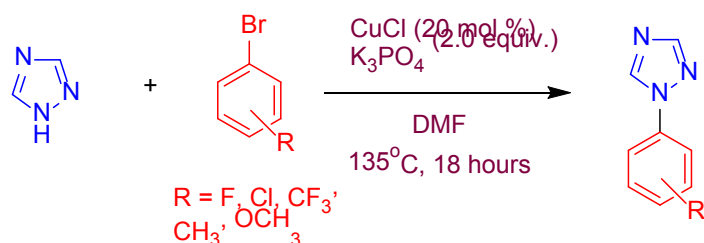
Abstract

N-aryl triazoles are an important and widely studied class of compounds due to their prevalence in numerous biologically active molecules and natural products. These heterocycles serve as key structural and functional motifs in pharmaceuticals, agrochemicals, and materials science, contributing to their broad range of applications.¹ The presence of the N-heteroaryl azole core in many bioactive compounds has driven significant research into the development of efficient and scalable synthetic methodologies to construct these frameworks. Although advancements in Ullmann-type reactions, such as the use of ligand systems², have reduced catalyst loading and enabled milder reaction conditions, these improvements come with challenges, including the high cost of ligands and the need for specially designed ligands in some instances. While aryl bromides are less reactive than aryl iodides, they are more affordable and less toxic, making them a preferable choice for a cost-effective and environmentally friendly approach. Moreover, catalytic methods for the ligand-free N-arylation of triazoles using aryl bromides remain limited.

In this paper³, we present a straightforward and practical method for the N-arylation of triazoles with various substituted aryl bromides, using CuCl (20 mol%) as the catalyst, K₃PO₄ as the base, and DMF under ligand free conditions. Under the optimised conditions, this method achieved moderate to good product yields, reaching up to 88%. The development of this methodology represents a step toward a more cost-effective and environmentally friendly strategy for the synthesis of N-arylated triazoles, offering potential applications in pharmaceutical and materials chemistry.

Keywords: triazole, copper(I) chloride, arylation, aryl bromides, ligand-free

Graphic / Image (Optional)



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POTENTIAL OF CHLOROALKENE AS PEPTIDE BOND ISOSTERE

Tetsuo Narumi^{a,b,*} Mio Takeda^a, Sayuri Takeo^b, Chihiro Iio^b, Ai Sakakibara^a

^a Graduate School of Integrated Science and Technology, Shizuoka University, Japan.

^b Graduate School of Medical Photonics, Shizuoka University, Japan.

*Corresponding author: narumi.tetsuo@shizuoka.ac.jp

Abstract

Replacement of a peptide bond with a peptide bond isostere is an established approach for increasing metabolic stability, potency, and selectivity. In particular, fluoroalkene dipeptide isosteres (FADIs) have been thought as one of the most ideal isosteres to mimic the shape and function of the ground state of peptide bonds and there are many reports on FADIs. On the other hands, chloroalkene dipeptide isosteres (CADIs) possessing the chlorine atom as the carbonyl oxygen equivalent have received less attention than FADIs, albeit with the advantages of the chlorine substituent as a bioisostere for many functional groups.

In our ongoing research to develop peptidomimetics, we have recently identified multi-gram preparative and diastereoselective synthetic strategies toward (Z)-CADIs.¹ In this symposium, we will present the synthesis of various peptidomimetics incorporating (Z)-CADIs using our established synthetic methods. We will discuss their applications as peptide bond isosteres in the design of bioactive peptides, including G4-binding peptides,² b-turn peptides,³ and hNMUR agonists.⁴ Additionally, we will explore the properties of these CADIs, including their potential to enhance cell permeability.⁵



Keywords: peptide bond isostere, b-turn, b-sheet, cyclic peptide, cell permeability

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SYNTHESIS AND STUDY OF SOME PHYSICOCHEMICAL CHARACTERISTICS OF NEW 1,8-NAPHTHALIMIDE-CONJUGATED HEMORPHIN ANALOGS

Petar Todorov^{a,*}, Stela Georgieva^b, Jana Tchekalarova^c,

^a*Department of Organic Chemistry, University of Chemical Technology and Metallurgy, Bulgaria*

^b*Department of Analytical Chemistry, University of Chemical Technology and Metallurgy, Bulgaria*

^c*Institute of Neurobiology, Bulgarian Academy of Sciences, Bulgaria*

**Corresponding author: pepi_37@abv.bg*

Abstract

The 1,8-naphthalimide dyes are widely used in medicinal and bioorganic chemistry as biologically active compounds alone or conjugated. Hemorphins in turn, are endogenous opioid peptides found in nature and are part of the hemorphin family. These peptides perform a variety of biological actions, including anticancer, antidiabetic, antihypertensive, and antiepilepsy. That is why we synthesized and physicochemically studied some novel 4-substituted-1,8-naphthalimides-conjugated hemorphin analogs, which could be sensitive fluorescent probes in biological applications. A modified solid-phase peptide synthesis via Fmoc-strategy was used, with 1,8-naphthalimides reacting directly to the resin with the N-terminal amino group to form the hemorphin analogs. The crude peptides were purified using an RP-HPLC, and their molecular weights were measured using ESI-MS. The aromatic peptide systems were evaluated for their conformational states, and anisotropy, as well as specific angles of optical rotation. The electrochemical properties were also discussed, and it was proven that some alterations in the amino acid skeleton affect the electrochemical behaviour of aromatic systems by affecting the reactivity of the redox function group. Furthermore, the compounds' second structures are studied using FT-IR and CD-dichroism to corroborate the conformational and anisotropy of these novel aromatic peptide systems. Moreover, the new compounds were evaluated for their antiseizure activity in the 6-Hz and maximal electroshock tests and in the pentylenetetrazol-induced seizure model in mice. They showed dose-dependent activity against psychomotor seizures, seizure spreading and suppressed clonic seizures in kindled mice, comparable to the reference drug diazepam.

Keywords: hemorphin, naphthalimides, opioid peptides, spectral analysis, anticonvulsant activity

Acknowledgment: This study is funded by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0002, "BiOrgaMCT".

SYNTHESIS AND EVALUATION OF 1,4-NAPHTHOQUINONE DERIVATIVES AS DNA INTERCALATING AGENTS

Nadezhda V. Danilenko^{a,*}, Andrei I. Khlebnikov^a

^a Tomsk Polytechnic University

*Corresponding author: nadezhda.dani@gmail.com

Abstract

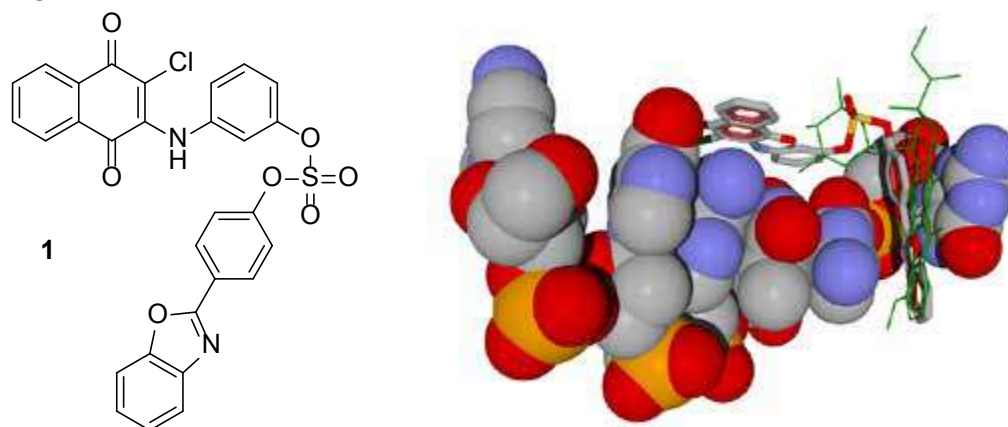
Naptoquinone derivatives possess anticancer activity [1], [2]. In this work, we have studied the compounds containing naphthoquinone and benzoxazole molecular scaffolds in their structures. Compound **1** (Figure 1) and its isomers with different positions of the sulfate group in the phenyl rings were synthesized via the SuFEx click reaction between fluorosulfate-containing 1,4-napthoquinone and 2-(hydroxyphenyl)benzoxazole derivatives.

Given that the known DNA intercalator doxorubicin contains an anthraquinone moiety, the compounds were expected to exhibit similar properties. To investigate the potential DNA-binding capabilities of the planar molecules, we performed molecular docking of compounds into the B-DNA structure (PDB: 151D) [3]. The binding region selected for the intercalation modeling corresponded to the doxorubicin binding site between guanine (G) and cytosine (C) base pair in the 151D structure. Molecular docking performed using the ROSIE server resulted in the position of compound **1** shown in Figure 1. In the optimal docking pose, compound **1** adopts a position analogous to the planar fragment of doxorubicin, with its benzoxazole moiety oriented toward the intercalation site. Additionally, compound **1** establishes a hydrogen bond between its NH-group and the oxygen atom of the thymine base.

The *in silico* study using molecular docking predicted anticancer potency of compounds through B-DNA intercalation, analogously to doxorubicin. The investigated compounds are of great interest for further studies as possible new anticancer agents.

Keywords: benzoxazole; 1,4-napthoquinone; SuFEx; anticancer activity

Figure 1



This research was supported by the Russian Science Foundation, project No. 24-15-00334.

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A SIMPLE MOLECULAR DESIGN STRATEGY FOR RED MULTIPLE RESONANCE EMITTERS

Haowen Chen^a, Wei Jiang^{a*},

^a School of Chemistry and Engineering, Southeast University.

*Corresponding author: jiangw@seu.edu.cn

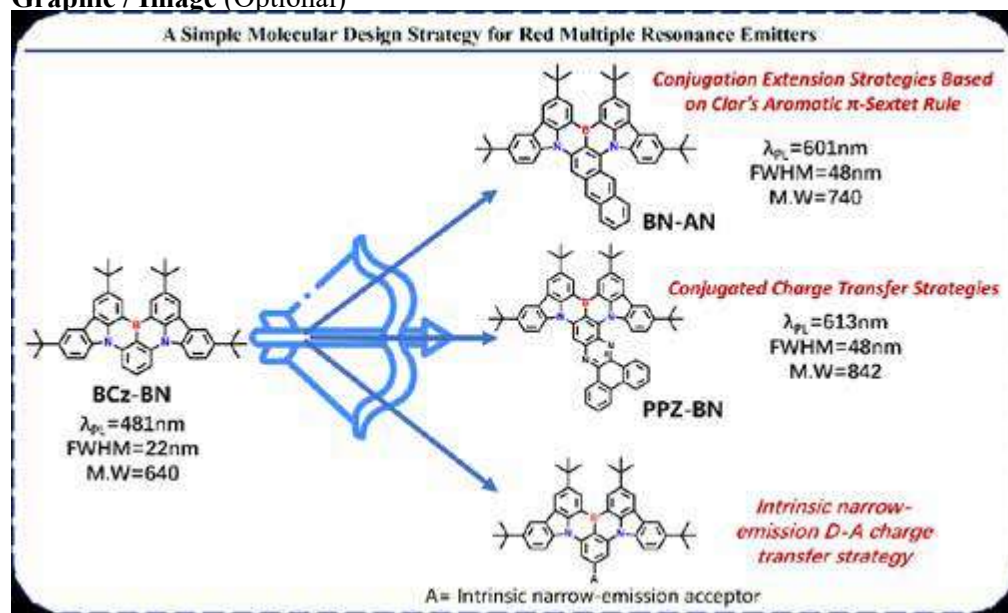
Abstract

Polycyclic heteroaromatics with multi-resonance (MR) characteristics are attractive materials for narrowband emitters in wide-color-gamut organic light-emitting diodes (OLEDs). Though the flourishing of materials with multiple resonance (MR) in blue to green regions, red emissive MR emitters are still rare in literatures, which definitely should be resolved for further applications. We have aimed at development of strategies for narrowband red-shifted emission and design narrowband red-emissive materials.

1. Conjugation Extension Strategies Based on Clar's Aromatic π -Sextet Rule (BN-AN)¹
2. Conjugated Charge Transfer Strategies (PPZ-BN)²
3. Intrinsic narrow-emission D-A charge transfer strategy

Keywords: organic light-emitting diodes, multiple resonance, narrowband red emission, π -conjugate extension.

Graphic / Image (Optional)



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EXPLORING THE INFLUENCE OF ELECTRONIC EFFECTS ON THE REACTIVITY OF PENTAFULVENES

Manisha Hota¹, Emma Keller¹, Todd Gillam², Chris Blencowe³, Anton Blencowe^{1*}

¹University of South Australia, Adelaide 5000, South Australia, Australia

²Murdoch University, Murdoch, Western Australia, 6150

³Fleet Bioprocessing, Hartley Wintney, Hampshire, United Kingdom, RG27 8DH

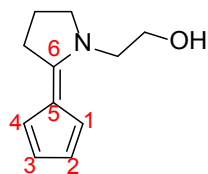
*Corresponding author: anton.blencowe@unisa.edu.au

Abstract

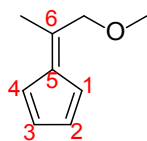
Pentafulvenes have been extensively studied due to their unique reactivity, which arises from their exocyclic double bond. Heterolytic cleavage of this bond generates aromatic and anti-aromatic zwitterionic intermediates that undergo efficient pericyclic reactions, distinguishing them from acyclic olefins and aromatic compounds. Previously, we reported the aqueous [4+2] cycloaddition of 6,6-dialkylpentafulvenes with maleimides as an effective biorthogonal conjugation strategy^{1,2}. Building on this work, we investigated the influence of different substituents on the reactivity of fulvenes with maleimides. Specifically, we studied the influence of resonance effects with an electron-donating group for a 6-aminopentafulvene and inductive effects with an electron-withdrawing group for a 6-(methoxymethyl)fulvene to assess how these electronic factors impact the type and rate of reactions with dienophiles.

The presence of an electron-donating amine group at the C6 position increased the nucleophilicity of the pentafulvene, with cyclopentadienyl protons undergoing rapid deuterium exchange in the presence of deuterium oxide, with significantly faster kinetics under acidic conditions and at the C1 and C4 positions. The reactivity of the 6-aminopentafulvene with dienophiles (e.g., maleimides) was highly solvent dependent. While no reaction was observed in low polarity solvents (e.g., chloroform), fulvene-mediated maleimide polymerisation dominated in dimethylsulfoxide and Michael addition occurred in water at the C1 and C4 positions consistent with the greater nucleophilicity at these positions. In contrast, reaction of the 6-methoxymethylfulvene with maleimides proceeded via a [4+2] cycloaddition regardless of the solvent, with faster reaction kinetics observed in polar solvents, such as water. These results highlight the significant influence of electronic effects on the reactivity of pentafulvenes.

Keywords: pentafulvene, dienophile, resonance effects, inductive effects



6-aminopentafulvene



6-(methoxymethyl)fulvene

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SHUTTTLING MOTION OF STIMULUSRESPONSIVE ROTAXANES WITH STERIC BARRIERS ON THE AXIAL COMPONENT

Masahiro Muraoka^{a*}, Hiroyuki Yoshimitsu^b, Shintaro Kawano^c, Motohiro Shizuma^{a,c}

^aFaculty of Engineering, Osaka Institute of Technology.

^bGraduate School of Engineering, Osaka Institute of Technology.

^cOsaka Research Institute of Industrial Science and Technology.

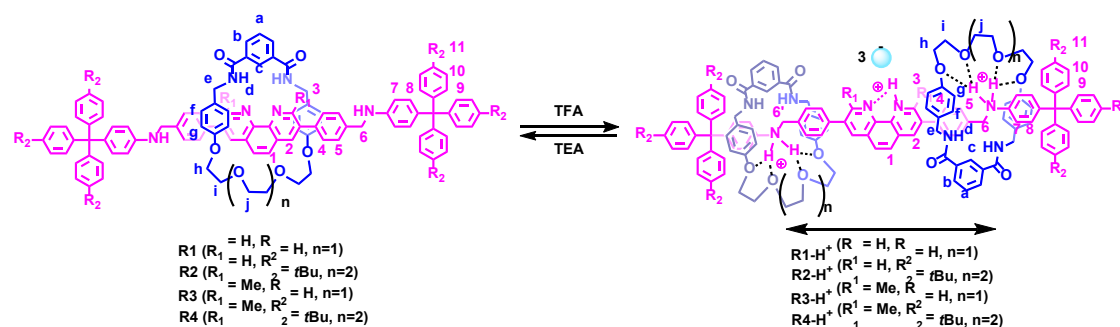
*Corresponding author: masahiro.muraoka@oit.ac.jp

Abstract

Rotaxane, known as a typical interlocked molecule, exhibits molecular shuttling and switching in response to external stimuli. Therefore, rotaxanes are expected to be applied to various molecular devices and molecular machines^{1, 2}. We have demonstrated the synthesis of [2]rotaxanes utilizing ring molecules composed of an isophthalic bisamide moiety with an oxyethylene chain and axis molecules consisting of a phenanthroline moiety, which showed molecular shuttling properties in response to acid as an external stimulus³⁻⁵.

In this study, we synthesized new [2]rotaxanes (**R3**, **R4**) with two methyl groups on a phenanthroline ring in the axial component as a steric barrier to compare with new [2]rotaxanes (**R1**, **R2**) without the substituents regarding the molecular dynamics of the shuttling motion. In addition, we compared the effect of the size of the ring component. After adding acid to the synthesized [2]rotaxanes, ¹H NMR measurements were performed to confirm the motion of the ring component. Under neutral conditions, the ring component remained at the phenanthroline moiety, and characteristic **Hc**, **Hf**, and **Hg** signal changes were observed. When phenanthroline and anilines were protonated by the addition of acid, the high-field shift due to the aromatic ring shielding was observed at the methylene group (**H6**) adjacent to the anilinium, suggesting that the ring component is close to the anilinium. Next, variable-temperature (VT) ¹H NMR measurements were performed to investigate the shuttling-related kinetics and energies. By comparing the obtained shuttling kinetics and shuttling energies, the presence of steric barriers was found to affect the molecular shuttling motion.

Keywords: stimuli-responsive rotaxanes, molecular shuttling, shuttling kinetic, shuttling energy, interlocked molecules.



Scheme 1. Molecular shuttling motions of [2]rotaxanes by acid-base.

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SELF-ADJUSTING α -HELICAL PEPTIDES ASSEMBLY FOR mRNA NANOTUBE FORMATION AND MAGNETIC CONTROL OF α -HELICAL PEPTIDE ASSEMBLY AND DISASSEMBLY

Zhihao Zhang^a, Sooho Ko^a, Shouqin Feng^a, Kyu-won Hwang^a, Jeongsu Park^a,
 and Yong-beom Lim^{a,*},

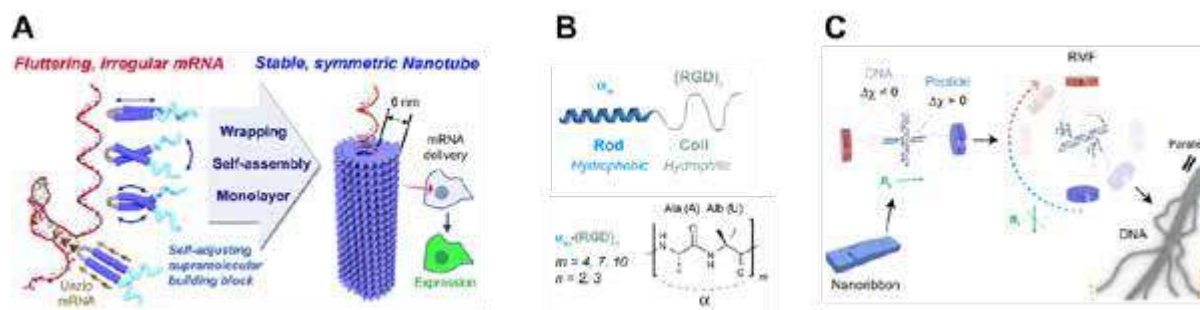
^aYonsei University, Seoul, Korea.

*Corresponding author: yblim@yonsei.ac.kr

Abstract

The success of mRNA vaccines has highlighted nucleic acid therapeutics, but challenges remain in safety, stability, and efficiency. Advanced delivery platforms are crucial to overcome these limitations. We introduce a novel nucleic acid delivery platform using self-adjusting α -helical rod-coil building blocks to overcome existing challenges in nucleic acid therapeutics. By incorporating self-adjusting building blocks (SABs), the platform enables the formation of mRNA nanotubes that can autonomously adjust their molecular structure to optimize interactions with nucleic acids. These nanotubes unravel secondary mRNA structures, coat nucleic acids into stable straight forms, and significantly enhance thermodynamic stability while protecting mRNA from enzymatic degradation. Moreover, ligand-bound mRNA nanotubes demonstrate high cellular uptake efficiency, and their protein expression levels can be finely tuned by adjusting the ratio of building blocks. Additionally, a magnetically responsive α -helical rod (MNP-helix) was developed to enable controlled self-assembly under an external magnetic field. This MNP-helix allows for the hierarchical coating and release of linear dsDNA, facilitating the creation of an artificial chromosome with controlled DNA release under a simple neodymium magnet. The integration of mRNA nanotube formation and magnetically responsive self-assembly holds great potential for the development of magnetically controllable mRNA nanotubes, paving the way for more precise and efficient nucleic acid-based therapeutics.

Keywords: nucleic acid delivery, self-assembly, peptide, stimuli-responsive materials.



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SELF-ASSEMBLED NANOPARTICLES: A STRATEGY TO OVERCOME THE PHARMACOKINETIC LIMITATIONS OF PEPTIDE THERAPEUTICS

Hyun Suk Hwang^a, Yong Beom Lim^{a,*}, Jung Yeon Ryu, Hye Soo Lee^a, Seung Jae Han^a

^aYonsei University.

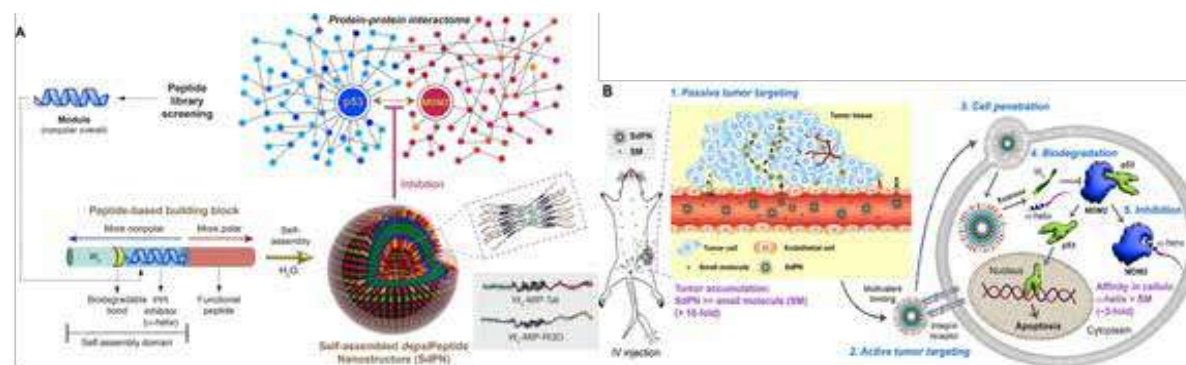
*Corresponding author: yblim@yonsei.ac.kr

Abstract

While peptides are known for their poor intrinsic pharmacokinetic properties, it is well-established that nanostructures with excellent pharmacokinetic profiles can be designed. Recognizing the typically nonpolar nature of peptide inhibitors, we have incorporated these inhibitors targeting intracellular protein–protein interactions (PPIs) into biodegradable self-assembled depsi-peptide nanostructures (SdPNs). In this design, the peptide inhibitor serves a dual role: inhibiting PPIs and facilitating self-assembly. This approach overcomes the challenges associated with the poor pharmacokinetics of peptides and the complications of encapsulation and entrapment processes. Optimized SdPNs exhibited superior tumor targeting and PPI inhibition capabilities *in vivo* compared to a comparable small molecule inhibitor. The kinetics of PPI inhibition by SdPNs were gradual and controllable, contrasting with the rapid inhibition kinetics of the small molecule. Due to the modular nature of SdPNs, any suitable peptide inhibitor can be incorporated into the platform, effectively bypassing the limitations posed by the poor pharmacokinetic properties of peptides

Keywords: PPIs, SdPNs, Platform, Poor pharmacokinetic property of peptides.

Graphic / Image (Optional)



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DISCOVERY OF NOVEL PYRIDINE DERIVATIVES AS A POTENTIAL HERBICIDE

So-Young Lee^{a,*}, Eunae Kim^a, Nam-Gyu Cho^b, Ki-Hwan Hwang^b, Young Kwan Ko^a, Suk-Jin Koo^b

^a*Korera Research Institute of Chemical Technology, KRICT*

^b*Moghu Research Center*

*Corresponding author: esso817@krikt.re.kr

Abstract

Herbicides are crop protection agents that inhibit or eliminate weeds without damaging crops. Among them, pyridine-based herbicides, such as Picloram, Fluroxypyr, Clopyralid, Aminopyralid, and Triclopyr, are widely used for crops like wheat, corn, and rice. However, existing pyridine-based herbicides have issues such as high application rates, complex production processes, and high manufacturing costs. So, the development of new herbicides is necessary. To address these challenges, we developed a novel pyridine-based herbicide. This herbicide contains an isoxazoline ring structure. This new formulation improves upon the limitations of conventional pyridine herbicides while maintaining excellent herbicidal performance.

The proposed herbicide effectively eliminates broadleaf weeds and demonstrates outstanding efficacy both before and after weed emergence. Additionally, its high selectivity ensures that it does not harm essential crops such as wheat, corn, and rice. Therefore, this research contributes to effective weed management and enhances agricultural productivity.

Keywords: herbicide, pyridine, isoxazoline, crop selectivity

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Rh(III)-CATALYZED C(sp²)-H ACTIVATION/ANNULATION FOR THE CONSTRUCTION OF PYRIMIDINYL-INCORPORATED PYRROLO[3,4-*b*] INDOLEDIONES

Yong Rok Lee^{a,*}, Muhammad Saeed Akhtar^a, Mohammad Aslam^a, Sonaimuthu Mohandoss^a

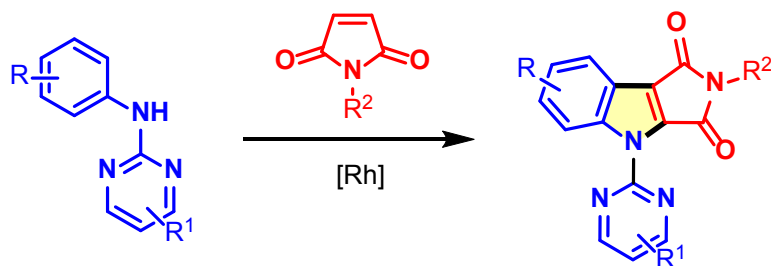
^a*School of Chemical Engineering, Yeungnam University, Gyeongsan 38541, Republic of Korea*

**Corresponding author: yrlee@yu.ac.kr*

Abstract

Indoles are a structurally diverse class of compounds with significant biological activity, which have attracted considerable attention in the fields of medicinal chemistry, natural product synthesis, and drug discovery. Ring-fused indoles are prevalent in various natural sources, such as plants, marine organisms, and microorganisms. They have demonstrated remarkable biological activities that make them attractive targets for drug development, including anticancer, antimalarial, antimicrobial, antiviral, anti-inflammatory, and neuroprotective activities. Among ring fused indoles, pyrrolo[3,4-*b*] indoles are widely found in drugs and bioactive molecules. While efficient synthetic methods for preparing pyrrolo[3,4-*b*]indoles have been well established, synthetic approaches for pyrrolo[3,4-*b*]indolediones have been less frequently reported. Herein, we present a facile and efficient synthetic protocol for construction of diversely functionalized pyrimidinyl-incorporated pyrrolo[3,4-*b*]indolediones via Rh-catalyzed C-H activation/annulation of N-arylpyrimidin-2-amines with maleimides (Scheme 1). Furthermore, we demonstrate the potential application of the synthesized compounds as fluorescent chemosensors.

Keywords: Rh-catalyzed reaction, C-H activation, pyrrolo[3,4-*b*]indolediones, fluorescent chemosensors



Scheme 1. Synthetic strategy for construction of diversely functionalized pyrimidinyl-incorporated pyrrolo[3,4-*b*]indolediones

SYNTHESIS OF DIHYDROPYRIMIDINE – TRIAZOLE, PYRAZOLO PYRIDINES AND *N*-HETEROCYCLE CHALCONES DERIVATIVES AS CANCER MDR AGENTS

Yeray Rodríguez-Núñez^{a,*}, Efraín Polo-Cuadrado^b, Glaucio Valdameri^c

^aUniversidad Andrés Bello, Departamento de Ciencias Químicas, Santiago 8370146, Chile

^bDepartamento de Química Orgánica, Universidad de Concepción, Concepción, Chile.

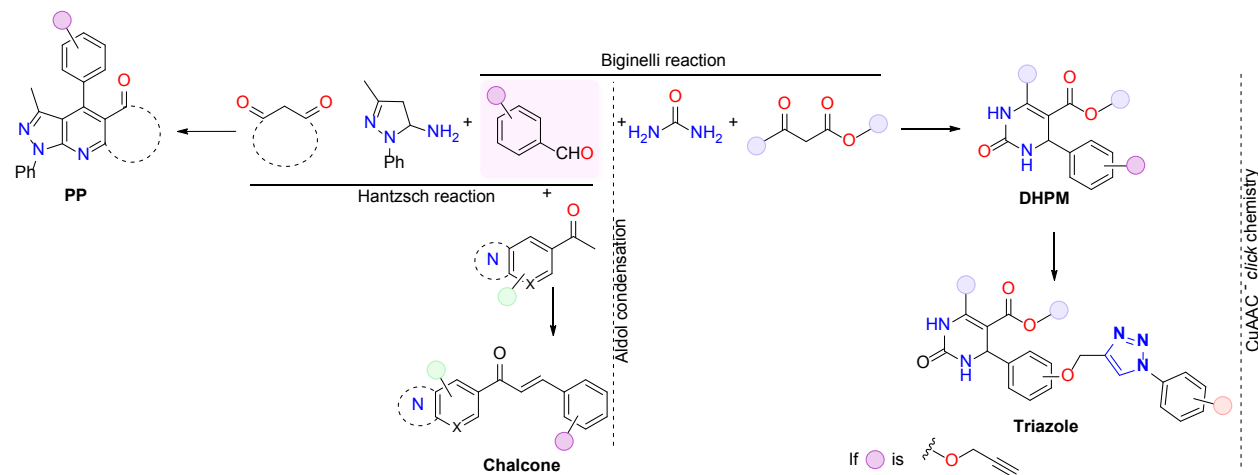
^cLaboratory of Cancer Drug Resistance, Federal University of Parana, Curitiba 80210-170, PR, Brazil

*Corresponding author: veray.rodriguez@unab.cl

Abstract

One of the most evident difficulties during chemotherapy processes is the development of multidrug resistance (MDR). In this context, drug resistance is mediated by ATP-binding cassette (ABC) transporters, including P-glycoprotein (P-gp), the breast cancer resistance protein ABCG2, and several isoforms of the multidrug resistance protein (MRP). In “classical MDR” tumor cells, the ABC transporter, P-glycoprotein, acts as an ATP-dependent multidrug efflux pump conferring resistance to many cytotoxic anticancer drugs and a variety of other hydrophobic compounds¹. The use of small molecules that have a potential inhibitory effect on these efflux pumps is one of the strategies to combat MDR in cancer². In this way, the design and synthesis of *N*-heterocycle compounds dihydropyridine-triazole, pyrazolo pyridines and α,β -unsaturated compounds (chalcones) through different synthesis methods such as Hantzsch reaction, Biginelli reaction, Aldol reaction, and click reaction was carried out and yield of reaction of each derivative series was among 60 and 90%. Likewise, using bioinformatic tools (Molecular docking, Drug-likeness calculation, and Molecular dynamics simulation) we can have a first approach about binding mode of this compounds and the stability in the active site of protein target. Preliminary results show that some *N*-heterocyclic chalcone derivatives and pyrazolopyridines inhibit the activity of some efflux pumps such as ABCG2 and MRP1, however, none of the compounds showed activity against P-gp, being selective towards the other two channels mainly, and some exclusively selective against MRP1.

Keywords: ATP binding cassette, Cancer, *N*-heterocycle synthesis, Inhibition efflux pump, bioinformatic tools,



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SYNTHESIS OF LUMINESCENT α,β -UNSATURATED OXADIAZOLES: DETERMINATION OF THEIR PHOTOPHYSICAL PROPERTIES

Eugenio Hernández-Fernández^{a,*}, Zuleyma Martínez-Campos^a, Susana T. López-Cortina^a,
Israel López^a, Mónica E. Anaya-Tamez^a, David J. Michaelis^b

^aUniversidad Autónoma de Nuevo León (UANL), Facultad de Ciencias Químicas (FCQ), San Nicolas
de los Garza, Nuevo Leon, Mexico

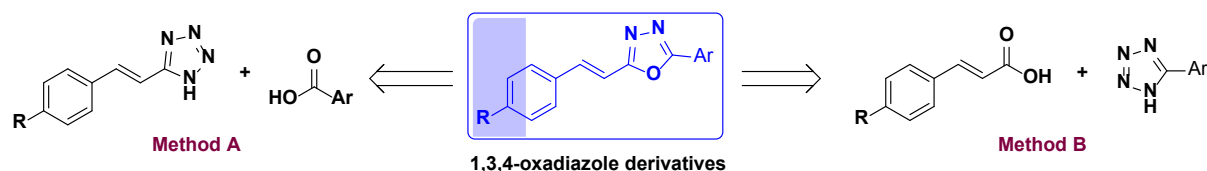
^bDepartment of Chemistry and Biochemistry, Brigham Young University, 84602, Provo, Utah, United States

*Corresponding author: eugenio.hernandezfr@uanl.edu.mx

Abstract

The design and synthesis of luminescent organic compounds incorporating a donor- π -acceptor system in their structure has gained significant interest in the field of materials chemistry due to their unique structural, photophysical, and electronic properties.¹ For example, this type of compounds has been used as selective sensors for metal ions,² as materials for OLED fabrication,³ as luminescent sensors in biomedical assays,⁴ among others. In this regard, 2,5-diaryl-1,3,4-oxadiazole derivatives have shown noticeable characteristics,⁵ and for this reason various research groups have focused their efforts on the synthesis of simple molecules using straightforward and environmentally friendly methodologies. In this work, we present the synthesis of low molecular weight 1,3,4-oxadiazole derivatives, assisted by microwave irradiation as a green alternative, following two methodologies. The first one involves the reaction between a derivative of an α,β -unsaturated tetrazole and aromatic carboxylic acids, achieving chemical yields between 30% to 80%. The second one involves the reaction between an α,β -unsaturated carboxylic acid and phenyl tetrazole, generating the oxadiazoles of interest with chemical yields from 60% to 90%. All the obtained compounds were found to be luminescent, and their photophysical properties were determined by UV-Vis and fluorescence spectroscopies, showing Stokes shifts (SS) greater than 80 nm and molar absorptivity coefficients (ϵ) greater than 25,000 M⁻¹cm⁻¹. These characteristics make them excellent candidates for their potential use in bioimaging generation.

Keywords: α,β -unsaturated oxadiazoles, luminescence, microwave, tetrazoles, organic synthesis.



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PEPTIDE SYNTHESIS IN AQUACULTURE: IL-8 DERIVATIVES FOR PATHOGEN CONTROL IN SALMON FARMING

Paula Santana^{a,*}, Constanza Guzmán^b, Nicolás Galleguillos^a, David Ramírez^c, Fanny Guzmán^d

^aInstituto de Ciencias Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Santiago, Chile.

^bCarrera de Química y Farmacia, Facultad de Salud, Universidad Autónoma de Chile, Santiago, Chile.

^cDepartamento de Farmacología, Facultad de Ciencias Biológicas, Universidad de Concepción, Concepción, Chile.

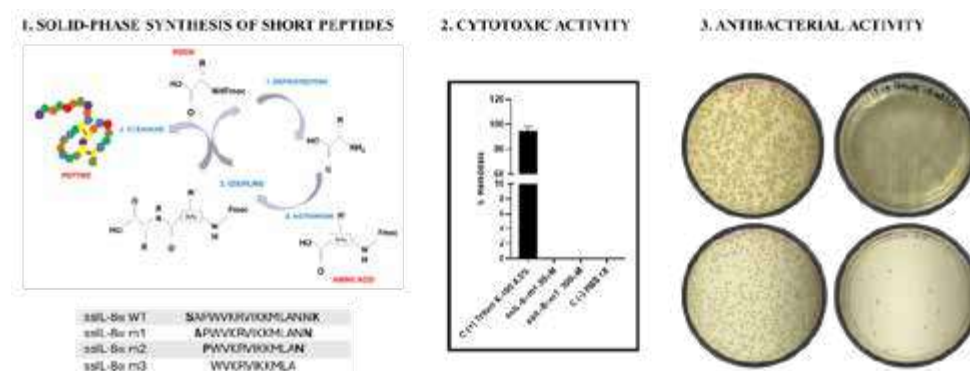
^dNúcleo Biotecnología Curauma (NBC), Pontificia Universidad Católica de Valparaíso, Valparaíso, Chile.

*Corresponding author: paula.santana@uautonoma.cl

Abstract

Chile, recognized as the second-largest salmon producer worldwide and contributing 31% to global production in 2024, faces significant challenges related to bacterial diseases affecting fish. These issues are linked to factors such as the physiological deterioration of salmonids, microorganism virulence, and environmental pollution¹. Traditional uses of vaccines and antibiotics have shown limitations, including questions about their effectiveness, the development of resistance, and residual contamination. In search of more sustainable alternatives, our research group has explored the use of host defense peptides, specifically peptides derived from the C-terminal end of the salmon IL-8 chemokine, known as ssIL-8 α . These compounds, consisting of 17 residues, exhibit promising antimicrobial properties². This work aimed to synthesize short peptides derived from IL-8 to preserve or enhance their antibacterial activity. Using the Fmoc methodology, we synthesized three peptides, which were characterized by reverse-phase HPLC, mass spectrometry, and circular dichroism, confirming a purity over 90% and structures of alpha-helix and random coil types. Their toxicity was assessed in erythrocytes and monocyte/macrophage cell lines at concentrations of 30 and 300 μ M, showing no cytotoxicity. The antibacterial activity was tested against *Escherichia coli*, *Staphylococcus aureus*, and *Aeromonas salmonicida*, demonstrating effectiveness at concentrations below 30 μ M. Additionally, these peptides inhibited up to 50% of biofilm growth of *A. salmonicida* between 10-25 μ M. These results suggest that ssIL-8 α -based antibacterial peptides could be an effective tool for controlling diseases in the salmon farming industry, reducing reliance on antibiotics and enhancing the productivity and sustainability of the sector.

Keywords: Fmoc synthesis, antimicrobial peptides, biofilm inhibition, interleukin 8, salmonids.



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A NOVEL HYDROXYPHOSPHONATES AS STIMULATORS OF PLANT GROWTH

Malmakova A.E.^{a,c*}, Otegulova K.B.^{a,b}, Nurlanuly N.^c

^a*Bekturov Institute of Chemical Sciences, Almaty, Kazakhstan.*

^b*Kazakh National Women's Teacher Training University, Almaty, Kazakhstan.*

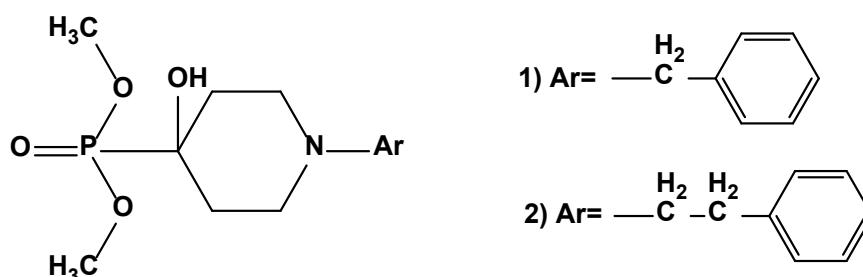
^c*Kazakh-British Technical University, Almaty, Kazakhstan.*

*Corresponding author: malmakova@mail.ru

Abstract

Preparing seed material for disinfection, protecting seedlings from external pathogenic factors and increasing resistance to them, and stimulating plant growth and development during the growing season and during seed germination using pre-sowing treatment with growth regulators - which can mobilize potential, genotypically determined plant capabilities - are some of the primary strategies for increasing grain yield. This study investigates the potential of novel hydroxyphosphonates as stimulators of plant growth. Hydroxyphosphonates **1**, **2**, characterized by their unique chemical structure, exhibit bioactivity that promotes plant development. Through a series of controlled experiments, we evaluated the effects of these compounds on height of plant and root elongation in various model samples of spring wheats *Triticum aestivum* *Kazakhstanskaya-10*, *Severyanka* and *Miras*. The *Kazakhstanskaya-10* was examined as a benchmark. The height of the wheat plant extends to 18,3 cm (25%), 16,77±1,64 (35%) and 16,12±1,16 (30 %) compared to the *Kazakhstanskaya-10*. Both hydroxyphosphonates significantly accelerated the growth and development of wheat seedlings of the three tested varieties: the roots increased by 18–22%. Results indicate that hydroxyphosphonates **1**, **2** significantly enhance growth parameters compared to control groups, suggesting their role in modulating physiological processes such as nutrient uptake and stress response. This research highlights the potential of hydroxyphosphonates as eco-friendly growth stimulators, offering a novel approach to sustainable agriculture and crop enhancement.

Keywords: hydroxyphosphonate, stimulator, plant growth



The research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (PTF IRN BR21882220 and GF IRN AP22685628).

THIAZOLE-SCHIFF BASE CONTAINING THIOSEMICARBAZONES: SYNTHESIS, ANTIMICROBIAL AND ANTIOXIDANT ACTIVITY WITH ADMET PREDICTION, MOLECULAR DOCKING STUDY AND DYNAMICS SIMULATION

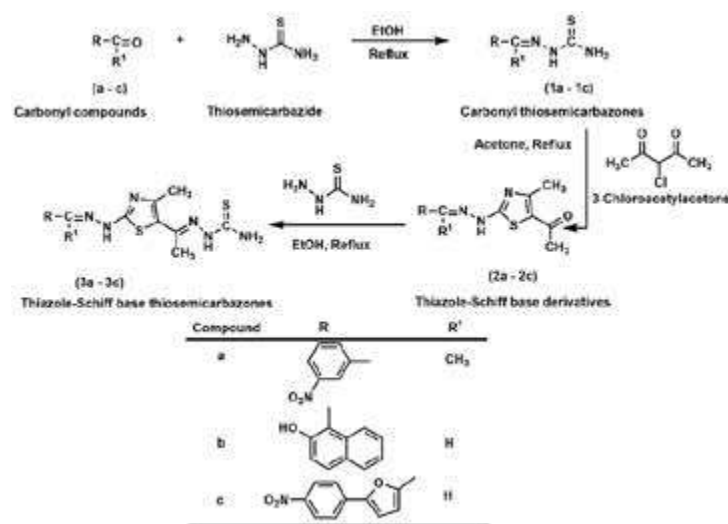
Md. Mizanur Rahman^{1*}, Mohammad Mostafizur Rahman¹, Md. Aminul Haque¹

¹Department of Chemistry, Jagannath University, Dhaka 1100, Bangladesh

*Corresponding author: chemizanphd@gmail.com

Abstract

In this study, three thiosemicarbazones (**1a-1c**), three thiazole-Schiff base derivatives (**2a-2c**), and three thiazole-Schiff base thiosemicarbazones (**3a-3c**) were synthesized (**Scheme 1**) through three consecutive reaction methods. The structures of the compounds were confirmed using various spectral methods, including IR, ¹H NMR, and HRMS. Among the synthesized compounds, 2-hydroxynaphthaldehydethiazole-2-thiosemicarbazone (**3b**) showed significant activity against all the fungal strains against six fungal strains. It demonstrated prominent antifungal activity against *Neurospora crassa* (45.5 ± 0.2 mm), *Aspergillus flavus* (42.6 ± 0.6 mm), *Candida albicans* (42.3 ± 0.5 mm), compared to standard amphotericin B (15.3 ± 0.5 mm, 11.3 ± 0.4 mm, and 16.7 ± 0.6 mm respectively). Moreover, compound **3b** also exhibited moderate antimicrobial activity against two Gram-negative bacteria and two Gram-positive bacteria, comparable to the standard ceftriaxone, as determined by the disc diffusion technique. The antioxidant activity of the synthesized analogues was assessed by DPPH free radical scavenging assay, in which **3b** displayed higher antioxidant activity (IC₅₀ = 35.73 ± 4.03 µg/mL) compared to the standard ascorbic acid (IC₅₀ = 40.47 ± 1.11 µg/mL). *In silico* studies indicated that the synthesized derivatives follow the Veber's rule and the Lipinski's rule of five. They also displayed good drug-likeness and drug-score properties. Moreover, the molecular docking studies of compound **3b** showed high binding affinities with target protein receptors. The simple synthetic pathways and enhanced biological activities of the synthesized analogues reported in this study could be beneficial for future drug discovery.



Scheme 1. Synthetic route for the synthesis of carbonyl thiosemicarbazones (**1a-1c**), thiazole Schiff-base derivatives (**2a-2c**), and thiazole-Schiff base thiosemicarbazones (**3a-3c**).

STEREODIVERGENCE IN CHALCOGEN AND HYDROGEN BOND-BASED ORGANOCATALYSIS

Jan Sokolov^a, Abhishek Bissoyi^a, Tomáš Hodík^{a*}

^a Charles University, Czechia

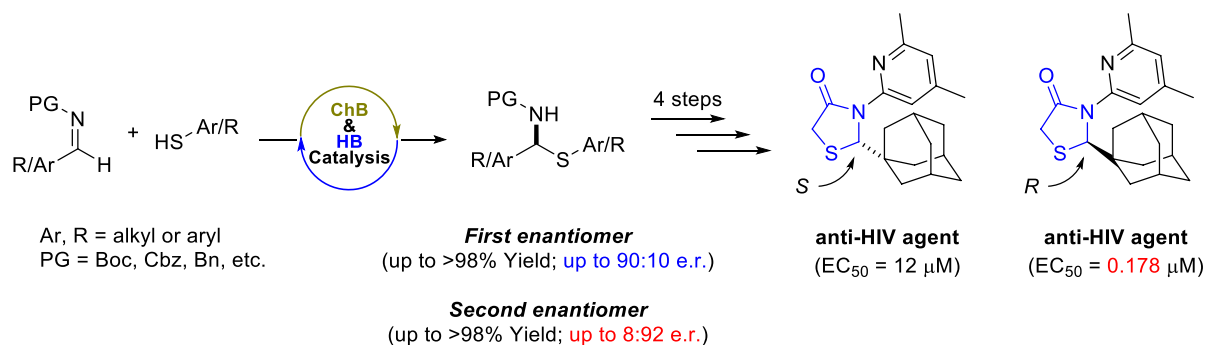
*Corresponding author: hodikt@faf.cuni.cz

Abstract

The art of accessing multiple stereoisomers from the same starting materials has been a keystone of modern organic chemistry. Numerous methods have been developed to control the stereodifferentiation event in a **stereodivergent manner**. However, the synthetic approaches based on well-tailored and distinct catalytic systems (mainly metal-based) still dominate the field.^[1] The importance of **stereodivergent synthesis is best demonstrated in the bioactivity of chiral thiazolidin-4-one** of which the chirality-dependent bioactivity has been undoubtedly proved.^[2] Within this project, we envision a conceptually new strategy for stereodivergent catalysis in which the stereodivergence is controlled in **pyramidal interconversion within a specific catalytic system**. Our novel catalytic system combines synergistically employed two diverse non-covalent interactions - **hydrogen and chalcogen bonding**. Moreover, the stereodivergentiation has been envisioned thanks to the inherent pyramidal interconversion of the chalcogen atom within a single catalytic system.

We are lucky to present the preliminary and not-yet optimized results declaring the feasibility of stereodivergent catalysis triggered exclusively by inherent pyramidal interconversion with **excellent yields** (up to >98%) and **great enantioselectivity** (up to 90:10 e.r. for the first enantiomer and up to 8:92 e.r. for the other one). All this has been achieved with a single catalyst with a switchable chiral pocket.

Keywords: stereodivergent synthesis, bifunctional organocatalysts, chalcogen bond, hydrogen bond, bioactive molecules



The Charles University (PRIMUS/22/SCI/015) and the Ministry of Education, Youth and Sports (Czech Republic) (CZ.02.01.01/00/22_008/0004607) are acknowledged for their generous support of this research.

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PERFLUORO ALKYL CHAIN INFLUENCE ON PHOTOPHYSICAL PROPERTIES AND MOLECULAR PACKING OF FLUOROPHORES

Chettukindhi Shirisha, Pin-Zong Lai, Jiayi Yang, Cheng-You Xu, Che-Jen Lin*

Department of Chemistry, National Dong Hwa University

*Corresponding author: chejen@gms.ndhu.edu.tw

Abstract

Fluorescent materials with aggregation-induced emission (AIE)¹ and *J*-aggregates have held significant attention due to their unique photophysical properties.^{2,3} This study explores the effect of alkyl chain length on the Photophysical properties and molecular packing of fluorophores, **1-R_FPy(C₈)**, **9-R_FAn(C₈)**, **2-R_FAn(C₈)** and **1-R_FPy(C₆)**, **9-R_FAn(C₆)**, **2-R_FAn(C₆)**. We have resolved the single crystals of **1-R_FPy(C₈)** and **9-R_FAn(C₈)** and **9-R_FAn(C₆)** found the F-F interactions play a crucial role in molecular packing. Replacing the bromine with semi-perfluoroalkyl groups enhances the fluorescent intensity in dilute solutions. The **1-R_FPy(C₈)** aggregates showed emission color variation from blue to green. Moreover, the **1-R_FPy(C₈)** powders exhibited stimuli-responsive emissions after THF-vapor fuming and grinding. However, the anthracene derivative **9-R_FAn(C₈)** only shows aggregation-caused quenched (ACQ).

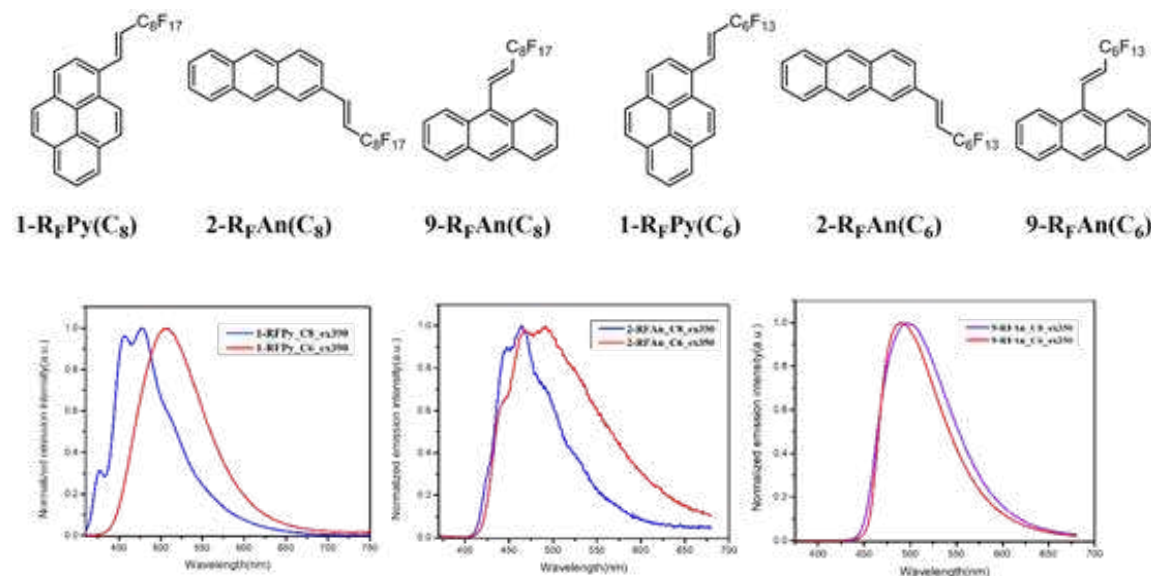


Figure 1. Solid state Emission behavior of semiperfluoroalkyl(C₈F₁₇ & C₆F₁₃) substituted chromophores

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EXPLORING PYRAZOLONE AZOMETHINE ANALOGUES: SYNTHESIS, X-RAY CRYSTALLOGRAPHY, BIOLOGICAL EVALUATION, AND *IN SILICO* STUDIES

Mohammad Sayed Alam,^{a,*} and Junaid Uddin Ahmed^b

^aDepartment of Chemistry, Jagannath University, Dhaka 1100, Bangladesh

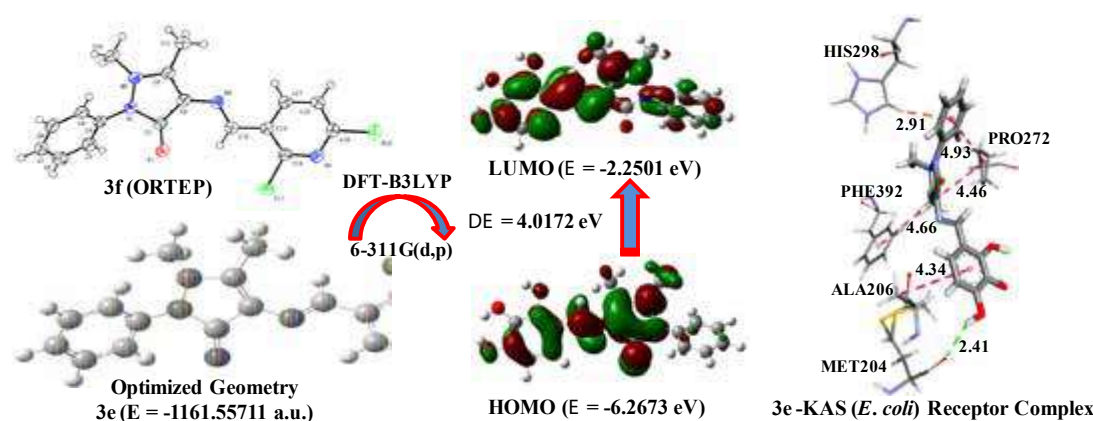
^bDepartment of Chemistry, Khulna University of Engineering and Technology, Khulna, Bangladesh

*Corresponding author: msalam@chem.jnu.ac.bd

Abstract

4-Aminoantipyrine (4-amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one, 4-AA) is a commercially available drug containing a pyrazolone moiety, known for its anti-inflammatory, analgesic, and antipyretic properties. The azomethine (–N=CH–) pharmacophore plays a pivotal role in its diverse bioactivities. In this study, a series of azomethine analogues (**3a–l**) derived from 4-AA were synthesized and characterized using FT-IR, ¹H-NMR, and EI mass spectrometry. Analogue **3f** was obtained as a single crystal, crystallizing in a monoclinic P2₁/n system with a *trans* C=N configuration. The crystal structure is stabilized by intermolecular C–H···O, C–H···π, and π···π interactions, forming a stacked supramolecular arrangement with four molecules per unit cell. *In vitro* antimicrobial screening against twelve bacterial and five fungal strains revealed weak to moderate activity for most analogues. Notably, **3a**, **3b**, **3e**, and **3g** exhibited strong bactericidal effects against *S. boydii*, *B. megaterium*, *S. sonnei*, and *E. coli*, respectively, while **3c**, **3d**, and **3l** showed potent fungicidal activity against *A. flavus*, *C. albicans*, and *N. crassa*. Antimicrobial efficacy was significantly influenced by the aromatic ring attached to the pyrazolone core via the azomethine (–C=N–) linker. DPPH radical scavenging assays demonstrated notable antioxidant activity for **3e**, **3l**, **3g**, **3k**, **3h**, and **3d**, with IC₅₀ values of 0.07, 1.19, 2.31, 2.57, 4.04, and 4.07 μg/mL, respectively, comparable to ascorbic acid (IC₅₀ = 4.10 μg/mL). Molecular docking studies revealed strong binding of the most active antibacterial (**3e**, **3g**) and antifungal (**3d**, **3l**) analogues to *E. coli* KAS and *C. albicans* CYP51 receptors, respectively. All compounds adhered to Lipinski's and Veber's rules, displayed favorable ADMET profiles, and showed potential as kinase, enzyme, and GPCR inhibitors in ligand-based target predictions. DFT calculations provided further insights into their molecular reactivity and biological properties.

Keywords: 4-Aminoantipyrine, Crystal structure, Azomethine analogue, Antioxidant, Anti-inflammatory, Cytotoxicity, Antimicrobial, Drug-likeness properties.



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MOLECULAR MECHANISM OF DIFFERENTIAL ALTERATION OF N-GLYCANS IN FROZEN-THAWED MEAT

Chang Wang^{a,*}, Minli Yang^a, Yun Ling^a, Muyi He^a,

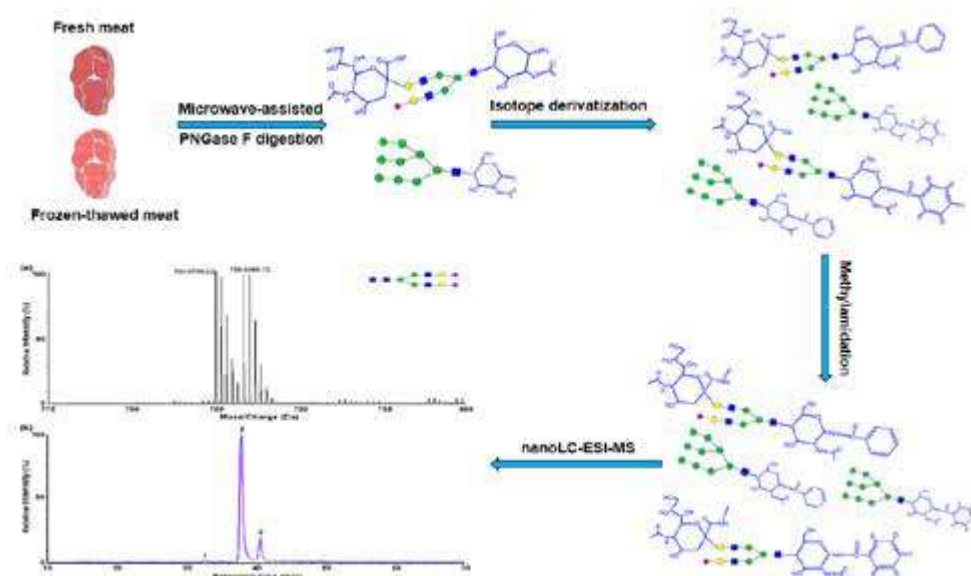
^a Chinese Academy of Quality and Inspection & Testing

*Corresponding author: beingwangchang@163.com

Abstract

The repeated freezing and thawing of raw meat will accelerate the degradation of proteins and loss of nutrients. However, previous detection technologies for identifying frozen-thawed meat are few, which are unable to effectively analyze the molecular mechanism in the process of freezing and thawing. Therefore, the establishment of frozen-thawed meat detection technology to screen novel biomarkers with high sensitivity and specificity is of great significance for in-depth analysis of the molecular mechanism of freeze-thaw changes and effective supervision of meat. In this study, dual-derivative strategies based on stable isotope labeling and methylation are proposed. Global profiling of N-glycans based on nanoLC-ESI-MS were established. These methods have possessed characteristics of high sensitivity, strong structural analysis capability and short time consumption, which overcome the shortcomings of traditional N-glycan analysis methods, such as low signal response, weak ability for branch and bond analysis, and long time consumption. By the proposed strategies, subtle changes of N-glycans in frozen-thawed meat were deeply analyzed from the perspective of isomeric profiling. Molecular model of differential changes of N-glycans in frozen-thawed meat are constructed and the molecular mechanism of related molecular changes are also explored. Eventually, specific biomarkers for identifying frozen-thawed meat can be screened. This project can provide novel ideas for the effective identification of frozen-thawed meat, and is of great significance to food safety.

Keywords: rapid detection, N-glycan, biomarker, frozen-thawed meat, specificity



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DESYMMETRIZATION OF CYCLOHEXADIENONES THROUGH PHASE-TRANSFER CATALYZED STEREOSELECTIVE INTRAMOLECULAR AZA-MICHAEL ADDITION WITH CHIRAL SULFINAMIDE NUCLEOPHILES

Bing-Syuan Wu^a, Tiow-Gan Ong^{a*}, Cheng-Che Tsai^{b*}

^a*Institute of Chemistry, Academia Sinica, Taipei, (Taiwan, ROC)*

^b*Department of Chemistry, Tunghai University, Taichung, (Taiwan, ROC)*

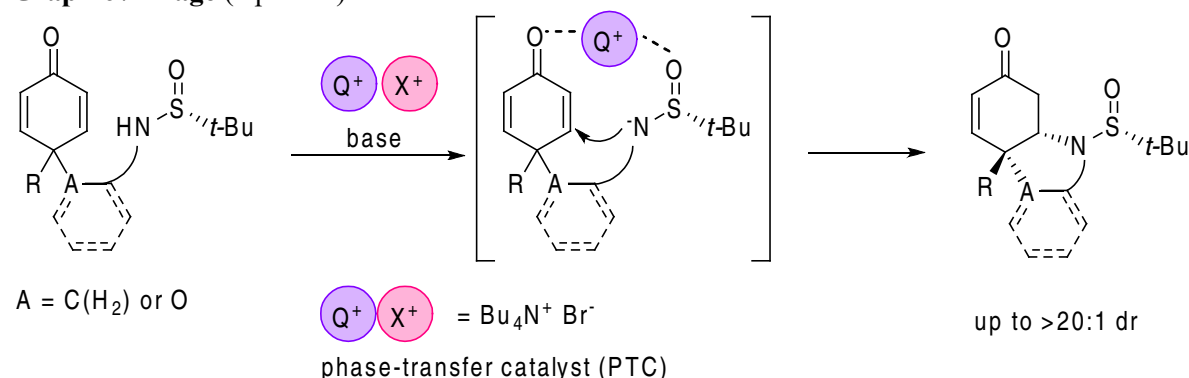
*Corresponding author: tgong@chem.sinica.edu.tw, chengchetsai@thu.edu.tw

Abstract

Building on the proven utility of *tert*-butyl sulfinamides (Ellman's reagents) in stereoselective aza-Michael additions,¹ this work extends their application to previously unexplored desymmetrization strategies for the synthesis of *N*-containing bicyclic frameworks,² which correspond to key structural motifs found in numerous bioactive natural products.³ The reaction proceeds through phase-transfer-catalyzed (PTC) intramolecular aza-Michael addition of chiral sulfinamide nucleophiles to cyclohexadienones, enabling the construction of chiral C–N bonds and affording products in up to 93% yield and >20:1 diastereomeric ratio, with confirmed absolute configuration and good scalability.⁴

Keywords: desymmetrization, chiral auxiliary, aza-Michael addition, PTC

Graphic / Image (Optional)



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PREDOMINANT COMPOUNDS OF *Neolitsea mollissima* ESSENTIAL OILS FROM TRAIL TO GUNUNG TANGGUNG (PAHANG AND PERAK BORDER), MALAYSIA

Mailina J^a, Nor Azah MA^{a*}, Saidatul Husni S^a, Mohd Shafik Yuzman T^b,
Nurliyana AL^c

^aForest Research Institute Malaysia (FRIM), 52109 Kepong, Selangor, Malaysia

^bDepartment of Chemistry Malaysia, Jalan Sultan 46661 Petaling Jaya, Selangor, Malaysia

^cHandcraft Tanah Rata, Jalan Besar, 39000 Tanah Rata, Cameron Highlands, Pahang, Malaysia

*Corresponding author: norazahmokhlis@gmail.com

Abstract

This work is aimed to examine the essential oil composition of an unexplored species, *Neolitsea mollissima*. The hydrodistilled essential oils of the leaves, fruits and twigs of *N. mollissima* were analyzed using GC-FID (retention indices RI) and GCMS. Thirty-seven compounds were found from this species with varied composition of chemical constituents from different plant parts. In this study, the leaf oils and twig oils were mainly dominated by sesquiterpenes: α -selinene representing (23.6%) and 1-*epi*-cubenol (15.9%) respectively. Chemical compounds present in appreciable amounts in the leaf oils were β -selinene (13.8%), (*E*)-nerolidol (9.2%), (*E,E*)- α -farnesene (2.6%) and δ -cadinene (2.7%) whereas the twig oils contained neo-intermedeol (14.9%), α -copaene (9.1%), α -terpineol (3.2%), viridiflorol (6.6%), pogostol (4.8%) and cubeban-11-ol (3.1%). Meanwhile, the fruit oils consisted of mainly monoterpenes of which δ -3-carene (28.0%), limonene (19.3%) and myrcene (16.5%) were the major compounds. Other compounds found in the fruit oils were α -selinene (8.6%), β -selinene (5.7%), selin-11-en-4- α -ol (6.8%) and γ -eudesmol (3.0%). To the best of our knowledge, this is the first chemical profiling study of *N. mollissima* found in Malaysia.

Keywords: essential oils, chemical profiling, *N. mollissima*, *neolitsea*

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FASTEN ROBOTIC SYNTHESIS OF BIOPOLYMERS BY AI GUIDED PREDICTION

Laura Russo^{a,b}

^aUniversità degli Studi di Milano Bicocca, Italy.

^bIRCCS Fondazione San Gerardo dei Tintori, Italy

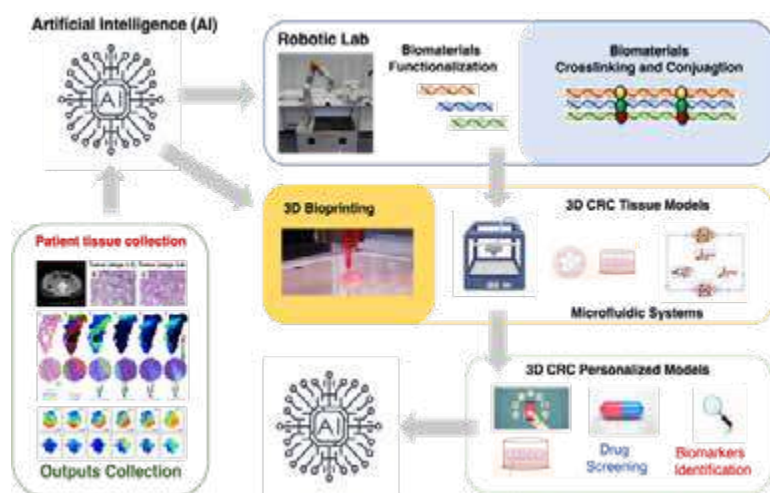
*Corresponding author: laura.russo@unimib.it

Abstract

The synthesis of biomaterials is fundamental for applications in biomedicine, tissue engineering, and drug delivery. In particular, the extracellular matrix (ECM) and its glycosignature play crucial roles in cell fate induction, including pathogenesis. The design of biomaterials that replicate the structural and biomolecular complexity of ECM, with particular emphasis of glycosignature, enables the creation of in vitro tissue models that replicate functional and structural features of human tissues [1-3]. The capacity to generate patient specific in vitro tissue models will allow to identify personalized therapeutic treatments. However, the high number of structural and biochemical variables to define and replicate, require the use of AI and the abandonment of artisanal approaches to fasten the research and limit human errors. Automated manufacturing systems and 3D bioprinting, integrated with Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL), can streamline the synthetic process, defining and tuning the structural and biomolecular properties of the construct, including the highly specific glycosignature, to generate the required personalized in vitro 3D tissue model.

This talk will present the development of AI-driven tools for the prediction and the automated synthesis of personalized 3D bioprinted tissue models, highlighting their potential to improve efficiency and predictive capabilities in biopolymer fabrication.

Keywords: Biomaterials; Glycocode; AI predictive synthesis, ECM mimics; Cell fate induction.



Acknowledgment: Financial support from: Iniziativa “PNC0000003 - “ANTHEM: AdvaNced Technologies for Human-centrEdMedicine”. CUP BICOCCA B53C2200667000; Ministero della Salute, RF-2021-12371959 Tackling immunomodulatory properties of stromal cells to improve therapeutic strategies in lung cancer. MUR PRIN 2022, 2022MY7AZT Dynamic multifunctional hydrogels for glioblastoma therapy (DINGO).

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AUTOMATION IN CHROMATOGRAPHIC SEPARATION

Fanyang Mo^{a,b,*}, Boxuan Zhao^a,

^a School of Materials Science and Engineering, Peking University, 100871, Beijing, P. R. China.

^b School of Advanced Materials, Peking University Shenzhen Graduate School, Shenzhen, 518055, China

*Corresponding author: fmo@pku.edu.cn

Abstract

Preparative column chromatography and preparative thin layer chromatography (TLC) are vital separation techniques in synthetic chemistry, yet they are hindered by high trial-and-error costs and labor-intensive, time-consuming procedures that reduce research efficiency. To alleviate these challenges, we are developing intelligent separation solutions using artificial intelligence (AI) and automation¹⁻³.

We have created comprehensive experimental platforms that automate the entire separation workflow. Our fully automated chromatography system handles all steps—from sample loading, fraction collection, pooling, and concentration to complete solvent removal. With a sample loading step, multiple samples are processed simultaneously to yield purified compounds. Similarly, our automated preparative TLC platform achieves precise spotting, high-throughput development, automated identification, scraping, and collection of sample spots from silica gel plates, greatly improving efficiency and safety.

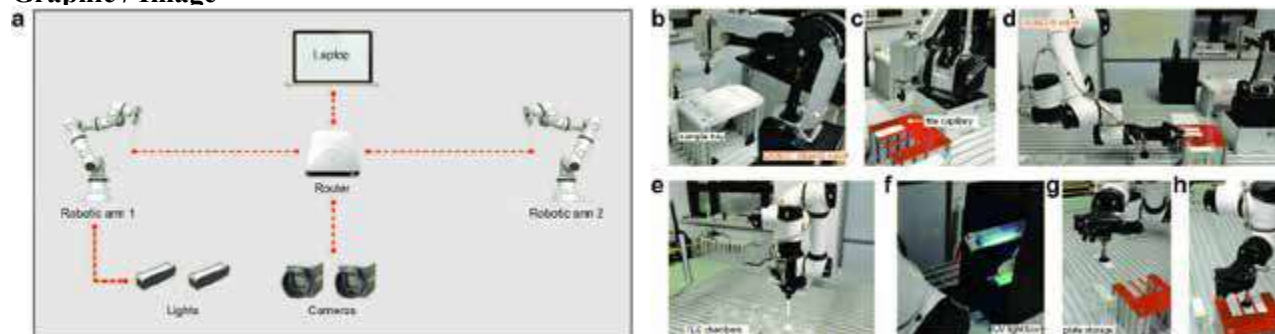
The high-quality data generated by these platforms enable us to tackle the complexities of chromatographic separations. Leveraging artificial intelligence, we can accurately predict outcomes for both TLC and column chromatography, significantly reducing the trial-and-error costs of optimizing conditions and advancing the process from automation to true intelligence. With integrated AI models, our column chromatography platform automatically determines optimal conditions based on the compounds, detects anomalies during separation, and promptly adjusts strategies to ensure stable, efficient purification. Concurrently, the automated TLC platform further enhances its intelligence by precisely predicting R_f values, facilitating automatic target identification and efficient collection.

This integrated approach not only streamlines the separation process but also improves reliability and throughput, ultimately advancing synthetic chemistry by allowing researchers to focus on innovation rather than routine operational tasks.

Keywords:

Preparative column chromatography; Thin layer chromatography; Artificial intelligence; Automation.

Graphic / Image



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TRANSFORMING SYNTHETIC CHEMISTRY WITH AN INTEGRATED HARDWARE-SOFTWARE AI CHEMIST SYSTEM

Kuangbiao Liao^{a,*}

^aGuangzhou National Laboratory, Guangzhou, China, 510000

*Corresponding author: liao_kuangbiao@gzlab.ac.cn

Abstract

The rapid development of automation, data science, and artificial intelligence (AI) is reshaping synthetic chemistry by addressing traditional challenges in efficiency, success rates, and safety. This presentation introduces an integrated hardware-software AI chemist system designed to automate project planning, experiment design, execution, data analysis, and modeling.

We have developed a modular, standardized high-throughput experimental (HTE) platform for rapid data collection and experimental optimization. Integrated with AI models and the specialized chemical language model SynAsk, the system uses extensive chemical databases and reasoning chains to optimize reaction paths, recommend conditions, and predict yields. The system's end-to-end capabilities include automated execution, AI-based modeling, and continuous optimization.

The integration of HTE with AI-driven models improves data collection efficiency and standardizes reaction conditions. The system has successfully discovered and optimized key chemical processes, such as hindered meta-C–H activation and iridium-catalyzed sulfoxonium ylides cross-coupling reactions. By combining AI, automation, and high-throughput technologies, it provides a comprehensive solution to the challenges in chemical research and offers a path forward for sustainable chemistry and drug discovery.

Keywords: AI Chemistry, HTE, Automation, Prediction Model, Large Language Model



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MATERIALEYES — SEEING THE INVISIBLE USING EXPERIMENT, THEORY, AND AI

Maria Chan

Center for Nanoscale Materials, Argonne National Laboratory

**Corresponding author: mchan@anl.gov*

Abstract

In the development of materials for realistic applications, the detection and understanding of atomic and electronic structures, especially of defects, interfaces, and nanostructures, is paramount. Advances characterization via electron, x-ray, and atom probes, in imaging, scattering, and spectroscopic modes, have brought us closer to such detection and understanding. However, such experimental data is often difficult to parse and relate to fundamental understanding of mechanisms and behavior at the atomic level. In this talk, I will discuss our efforts in MaterialEyes to use AI/ML and theoretical modeling to enable the seeing of atomic structures from experimental characterization data. I will also discuss our work in using AI to extract and use microscopy and spectroscopy data from scientific literature, and in developing data standards for materials science.

MOLEPRINTER: FULL AUTOMATIC WORKSTATION OF REPETITIVE SYNTHESIS

Changxu Lin^{a,b,*}

^a State Key Laboratory of Physical Chemistry of Solid Surface, Xiamen, China.

^b College of Physical Science and Technology, Xiamen University, China.

*Corresponding author: lincx@xmu.edu.cn

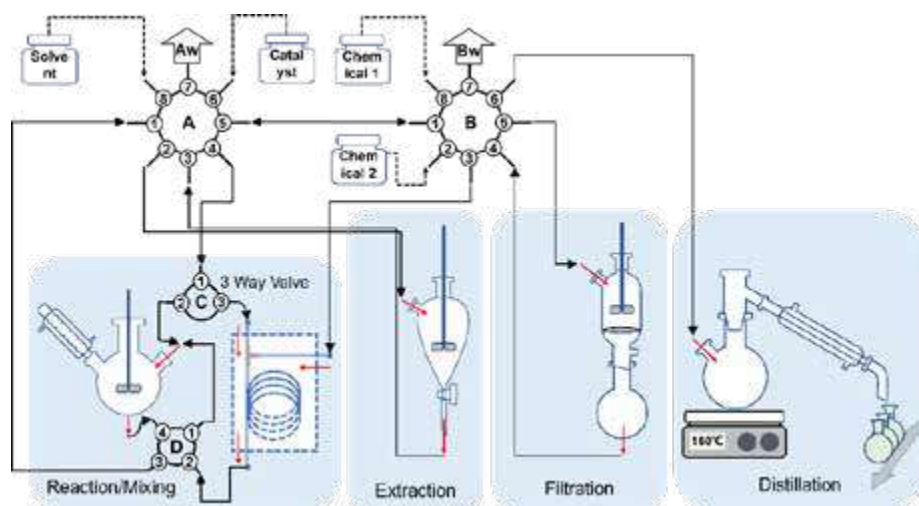
Abstract

Auto-synthesis Workstation (MPT) consists of various modules, including a central control module, liquid drive core, reaction module, extraction module, and drying module. The entire system standardizes different processes of chemical synthesis into modular components. By combining software with automated hardware equipment, the workstation integrates bottled reagents, three-neck flasks, separatory funnels, Buchner funnels, sintered glass funnels, mechanical stirrers, and various sensors. The core of the system—the pump valve core, composed of pipelines, syringe pumps, and valves enables the basic operations of automated chemical synthesis.

Its key features are:

- **Safety:** The fundamental value of automation in laboratories is to free personnel from manual tasks, reducing the risk of accidents caused by human error. It also helps avoid prolonged exposure to toxic and harmful substances, thereby ensuring the basic safety and health of laboratory staff.
- **Efficiency:** Compared to traditional manual synthesis, the MPT molecular printer can perform continuous synthesis work 24 hours a day based on programmed routines. It eliminates a large number of intermediate transfer operations, significantly increasing the yield of target molecules per unit of time and saving substantial labor and associated costs.
- **Stability:** The target molecules produced by the automated system have relatively stable yields and purity between batches, with no fluctuations in quality due to human operational errors. The experiment will strictly control reaction parameters such as reactant quantities, heating temperature, and heating duration according to the programmed values, ensuring that each reaction follows a completely consistent procedure and the product remains stable.

Keywords: Intelligent chemistry; Chemical automation; Experimental teaching; Comprehensive ability



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IS π -SINGLE BONDING (C– π –C) POSSIBLE? A CHALLENGE IN ORGANIC CHEMISTRY

Manabu Abe

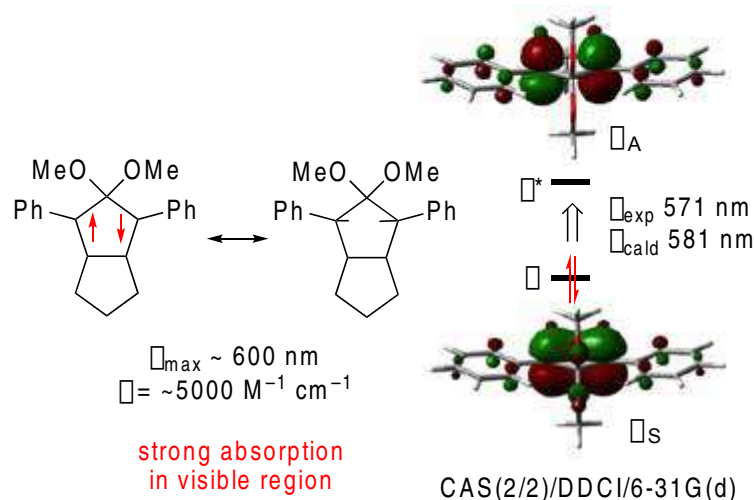
Department of Chemistry, Hiroshima University

*Corresponding author: mabe@hiroshima-u.ac.jp

Abstract

Chemical bonding systems determine the nature of molecules. In organic chemistry, there are two bonding types for carbon–carbon connections: σ -bonding and π -bonding. In this presentation, several aspects of studies in the last two decades addressing the naive question “Is π -single bonding (C– π –C) possible?” will be presented: (1) features of π -single bonded species; (2) molecular design for π -single bonding; (3) generation and detection of singlet diradicaloids with a π -single bonding character; (4) future prospects of π -single bonded species.

Keywords: π -single bonding, near-infrared light response, small HOMO-LUMO gap



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CONTROLLING MULTIPLE SELECTIVITIES IN RADICAL–RADICAL COMBINATIONS

Chao Zheng*

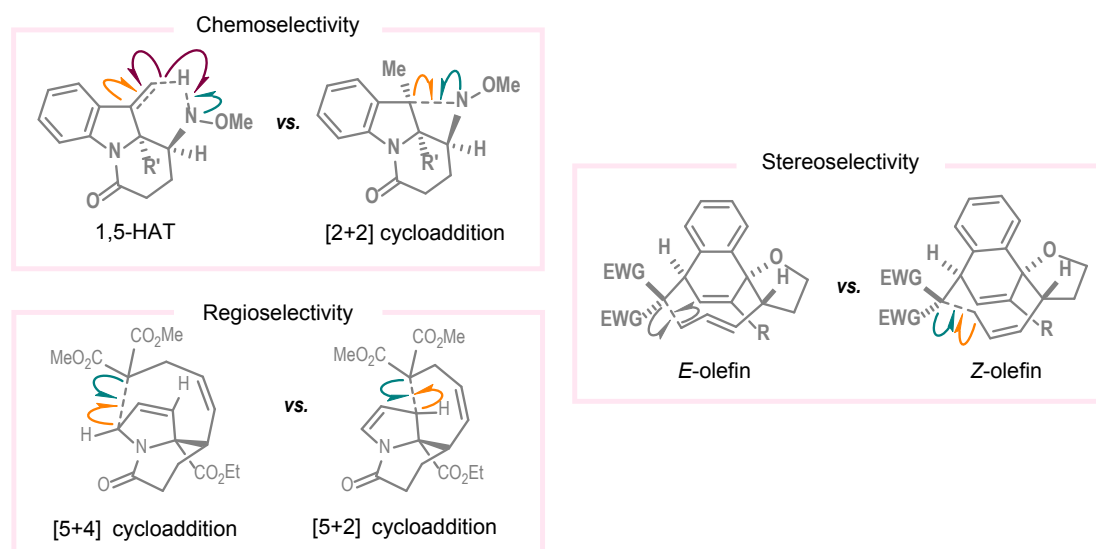
State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry,
Chinese Academy of Sciences, 345 Lingling Lu, Shanghai 200032, China

*Corresponding author: zhengchao@sioc.ac.cn

Abstract

Radical–radical combinations are among the fastest reactions in organic chemistry.¹ Thus, efficient synthesis of complex polycyclic molecules with radical–radical recombination as the key step, meanwhile achieving high level of chemo-, regio-, and stereoselectivity is quite challenging. In this talk, we will report our recent studies on visible-light-induced dearomative cycloaddition reactions of indole- or naphthalene-derivatives via Dexter energy-transfer mechanism.² In these reactions, the intramolecular 1,*n*-biradical recombination serves as the key step for the final carbon–carbon bond-formation. Systematic theoretical studies revealed thermodynamic, kinetic, or dynamic effects that dictates the multiple selectivities. These results provide new mechanistic insights into the synthetic reactions involving radical species, as well as powerful methods towards target molecules with increased complexity.

Keywords: dearomatization, energy transfer, radical–radical recombination, visible-light-catalysis



Radical–radical combination reactions with high selectivity

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THE INFLUENCE OF BRIDGE STATES ON THE EXCHANGE INTERACTION IN BIS-TRIARYLAMINE BIRADICAL DICATIONS

Leon Euringer^a, Marco Holzapfel^a, Ivo Krummenacher^{b,c}, Michael Franz^d, Sabine Richert^d, Holger Braunschweig^{b,c}, Christoph Lambert^{a,e,*}

^a*Institut für Organische Chemie, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.*

^b*Institut für Anorganische Chemie, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.*

^c*Institute for Sustainable Chemistry & Catalysis with Boron, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.*

^d*Institute of Physical Chemistry, University of Freiburg, Albertstraße 21, 79104 Freiburg, Germany.*

^e*Center für Nanosystems Chemistry, Universität Würzburg, Theodor-Boveri-Weg, 97074 Würzburg, Germany.*

**christoph.lambert@uni-wuerzburg.de*

Abstract

The influence of the electron density of a bridge connecting two redox centers on the magnetic super-exchange was investigated in a series of bridged bis-triarylamine mono- and dications. In this series, the bridge was 2,7-fluorenyl, where the bridge electron density was modified by substituents at the 9-position. For the dicationic biradicals, the singlet-triplet gap (exchange interaction) was determined by temperature dependent EPR spectroscopy and by quantum chemical methods. Hereby, an increase of antiferromagnetic coupling with a lowering of the bridge state energy by electron donating substituents was observed. Analysis of the involved molecular orbitals suggests that the ferromagnetic coupling is inversely proportional to the square of the bridge energy, which is also supported by the experimental findings. Thus, variation of the bridge state energy provides a design guideline for fine-tuning the properties of electronically coupled organic redox dyads.

Keywords: triarylamine, exchange interaction, EPR

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HETEROLE-FUSED DIBENZO[*a,f*]PENTALENES: DIRADICAL CHARACTER CONTROLLING BOND-SHIFT VALENCE TAUTOMERIZATION

Akihito Konishi*, Tomohiro Oda, Yusuke Mizuno, Makoto Yasuda*

Department of Applied Chemistry, Graduate School of Engineering, Osaka University

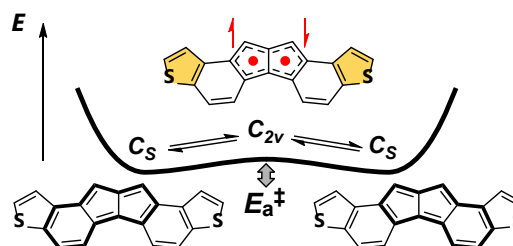
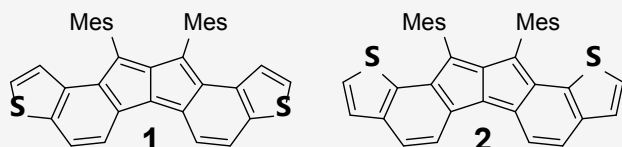
*Corresponding author: a-koni@chem.eng.osaka-u.ac.jp, yasuda@chem.eng.osaka-u.ac.jp

Abstract

Although the pseudo Jahn-Teller effect (PJTE)¹ is an essential effect to provide the attractive characteristics of $4n\pi$ systems, an understanding of the structure–property relationship derived from the PJTE for planar $4n\pi$ electron systems is still in its infancy. Herein, we describe the synthesis and characterization of two regioisomers of the thiophene-fused diareno[*a,f*]pentalenes **1** and **2**.² The magnetic and optoelectronic properties characterize these sulfur-doped diareno[*a,f*]pentalenes as open-shell antiaromatic molecules. Notably, thiophene-fused diareno[*a,f*]pentalenes **1** and **2** showed pronounced antiaromaticity, the strongest among our related systems,³ as well as moderate open-shell characteristics. Our experimental and theoretical investigations concluded that these properties are derived from the small energy barrier $E_a^\ddagger$ for the bond-shift valence tautomerization. The energy profile of the single crystal of **1** showed the temperature-dependent structural variations assigned to the dynamic mutual exchange between the two C_s -symmetric structures, which was also supported by changes in the chemical shifts of variable-temperature ¹H NMR spectra in the solution phase. The findings of this study advance the understanding of antiaromaticity characterized by the PJTE by controlling the energy barrier for bond-shift valence tautomerizations, potentially leading to the rational design of optoelectronic devices based on novel antiaromatic molecules possessing the strong contributions of their high-symmetric geometries.

Keywords: pentalene, antiaromaticity, diradical character, bond-shift valence tautomerization, pseudo Jahn-Teller effect

This work: dibenzothieno[*a,f*]pentalenes



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A PLUMBA-TRIPLET CARBENE AND PHOTOPHYSICS WITH CARBENE-BASED DIRADICALOIDS

Dominik Munz^{a,*}

^a Saarland University, Coordination Chemistry, D-66123 Saarbrücken, Germany.

*Corresponding author: dominik.munz@uni-saarland.de

Abstract

In this lecture, I will present on our recent progress toward stabilizing triplet carbenes through decoupling due to a heavy element, namely lead.¹ Further, I will review our contributions on how to stabilize singlet diradicaloids by carbenes, and how to apply these molecules as singlet-fission molecules.²⁻⁶ Eventually, current work on related text-book mixed-valence compounds and their photophysical properties will be discussed.

Keywords: Triplet Carbene, Diradicals, Conjugated Materials, Singlet Fission, Mixed-Valence Compounds

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MOLECULAR CARBONS WITH DIFFERENT SHAPES AND SIZES

Chunyan Chi*

Department of Chemistry, National University of Singapore

*Corresponding author: chmcc@nus.edu.sg

Abstract

Carbon-based nanostructures have shown revolutionary influence in the area of chemistry, physics and materials science. Recent efforts have been focused on novel topological structures of sp^2 -carbons such as carbon nanohoops, nanobelts, molecular cages, and open-shell nanographenes, which provoked new chemistry and materials. However, synthesis of this kind of molecules is extremely challenging mainly due to strain or intrinsic high reactivity. Another issue is that most of these carbon nanostructures have a localized aromatic character; that means, the π -electrons are not globally delocalized along the backbone, which limits their optical and electronic properties and applications. Herein, the synthesis of a series of novel pi-structures with different topologies will be introduced, and their physical properties, aromaticity and diradical character will be discussed. Some structures are shown in Figure 1.

Keywords: acenes, *peri*-acenes, carbon nanobelts, diradicaloids, aromaticity

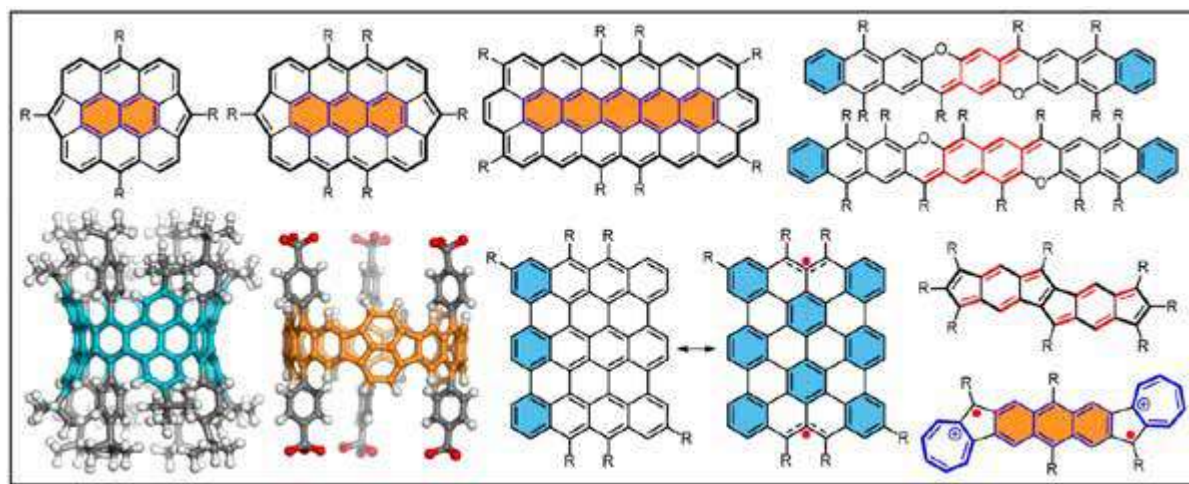


Figure 1. Some examples of pi-structures made in Chi group.

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THE TAMING OF *m*-XYLYLENE TYPE SINGLET DIRADICALOID BY DISPERSION FORCE

Yoshito Tobe^{a,b,*}, Jin-En Hung^a, Rumi Ozawa^b, Hsin-Chung Lin^a, Yogajivan Rout^a,
 Yutaka Ie^b, Yen-Ju Cheng^a

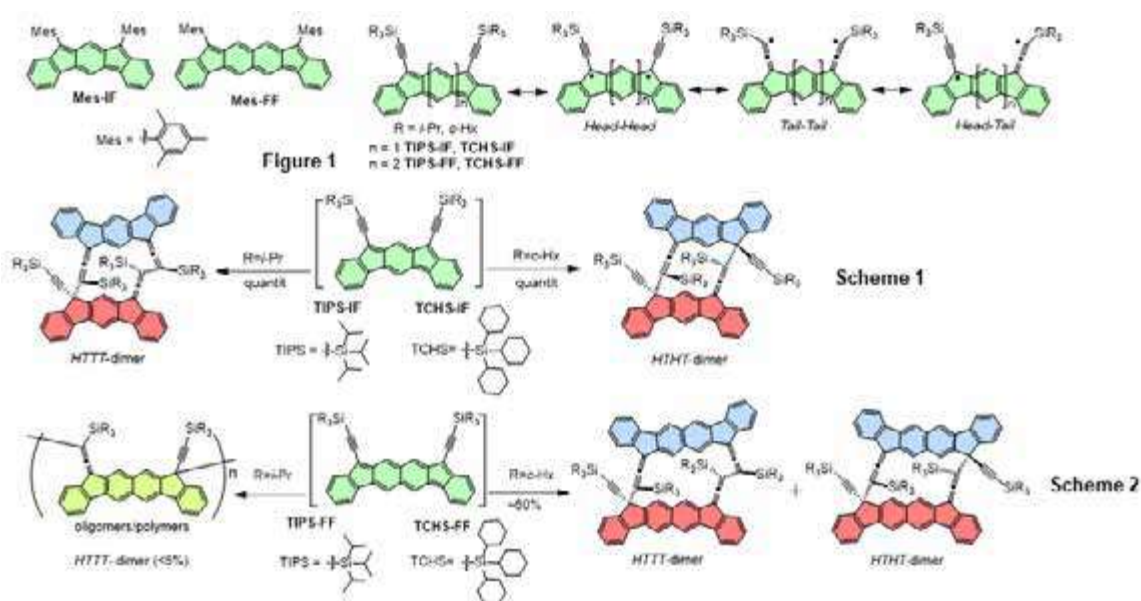
^a National Yang Ming Chiao Tung University, ^b Osaka University

*corresponding author: tobe@nycu.edu.tw

Abstract

We have reported the isolation and characterization of kinetically stabilized indeno[2,1-*b*]fluorene **Mes-IF** and its homolog fluoreno[2,3-*b*]fluorene **Mes-FF**, which are formally *meta*-xylylene type diradicaloids embedded in polycyclic frameworks, to reveal that they possess singlet ground state configurations with considerable open-shell character (Figure 1).^{1,2} To extend the scope of diradicaloids of this type, we examined the synthesis (trialkylsilyl) ethynyl derivatives with bulky isopropyl (**TIPS-IF** and **TIPS-FF**) and cyclohexyl (**TCH-IF** and **TCH-FF**) groups by SnCl₂-mediated reductive dehydroxylation of the corresponding dihydrodiols. Though none of the diradicaloids were isolated, we found that cyclic dimers were formed efficiently in all cases but one. Moreover, not only the reaction pathway (dimerization vs. oligomerization) but also the different dimer structures arising from the different sites of reaction (*Head* vs. *Tail*) are dependent on the alkyl groups. Namely, **TIPS-IF** and **TCH-IF** gave almost exclusively *HTTT* and *HTHT* dimers, respectively, furnishing products of distinct structures (Scheme 1). On the other hand, whereas **TIPS-FF** gave intractable oligomers/polymers mainly with only a trace amount of *HTTT* dimer, **TCH-FF** yielded dimers as the major product (60% yield, *HTTT* : *HTHT* = 2 : 1), formed through different reaction pathways (Scheme 2). The results indicate apparent yet delicate manifestation of London dispersion force to control reactive species.³

Keywords: *m*-xylylene, indenofluorene, diradicaloid, cyclodimerization, London dispersion force



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OPEN-SHELL ELECTRONIC STRUCTURES AND PROPERTIES OF π -STACKS OF DIRADICALOIDS

Ryohei Kishi^{a,b,c,*}, Wataru Yoshida^a, Kenji Okada^a, Hajime Miyamoto^a,
Ryota Sugimori^a, Kohei Tada^a, Yasutaka Kitagawa^{a,b,c,d}

^a*Graduate School of Engineering Science, Osaka University.*

^b*Center for Quantum Information and Quantum Biology (QIQB), Osaka University.*

^c*Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (ICS-OTRI),
Osaka University.*

^d*Spintronics Research Network Division, Institute for Open and Transdisciplinary Research Initiatives (OTRI-Spin),
Osaka University*

*Corresponding author: kishi.ryohei.es@osaka-u.ac.jp

Abstract

In this presentation, we will introduce our recent research studies on open-shell electronic structures and properties of π -stacks of diradicaloids where the strengths of through-bond and through-space (TB and TS) interactions are comparable. We developed theories, computations, and analysis methods based on the valence bond (VB) and molecular orbital (MO) theories for understanding the stacking structure dependences of open-shell electronic structures and properties of several π -stacks consisting of diradicaloids with various diradical characters (γ).

The developed theories help explore several interesting electronic structures that can be achieved by designing the TB/TS hybrid conjugated systems composed of diradicaloid molecules. For example, we derived conditions for achieving high diradical characters (i.e., narrow HOMO-LUMO gaps) in π -stacked n -mers, even consisting of monomers with weak diradical characters.¹ Since tuning the open-shell characters is critical to achieving highly efficient response properties, the obtained results and the developed theories will contribute to establishing design strategies for novel open-shell functional molecular materials.

Keywords: diradical molecule, π -stacked multimer, quantum chemical calculation, through-space conjugation

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THEORETICAL STUDY OF ELECTRON CONDUCTIVITY OF OPEN-SHELL SYSTEM AND ITS APPLICATION

Yasutaka Kitagawa^{a,b,c,d,e*}, Naoka Amamizu^a, Mitsuhiro Nishida^a,

Ren Inoue^a, Kaito Taka^a, Kohei Tada^a, Ryohei Kishi^{a,b,c,d}

^a Graduate School of Engineering Science, Osaka University.

^b Center for Quantum Information and Quantum Biology (QIQB),
International Advanced Research Institute (IARI), Osaka University.

^c Research Center for Solar Energy Chemistry (RCSEC),
Graduate School of Engineering Science, Osaka University.

^d Innovative Catalysis Science Division,
Institute for Open and Transdisciplinary Research Initiatives (ICS-OTRI), Osaka University.

^e Spintronics Research Network Division,
Institute for Open and Transdisciplinary Research Initiatives (OTRI-Spin), Osaka University.

*Corresponding author: kitagawa.yasutaka.es@osaka-u.ac.jp

Abstract

Microfabrication technology for integrated circuits has been developed according to Moore's Law. However, it has been suggested that the miniaturization of silicon (Si)-based devices has been almost reaching its limit. As an alternative to this "top-down approach", the use of single molecules for electronic components has attracted much attention as a "bottom-up approach". Since a theoretical proposal of a molecular rectifier in 1974, various functional single-molecule components such as molecular wires, transistors or switches and diodes have been proposed. To realize such single-molecular components, we focus on the open-shell nature of the molecules. For example, our group proposed that some of the extended metal atom chains (EMACs) can be used as the single molecule transistor controlled by an external magnetic field.¹⁻³ On the other hand, we also suggested that the open-shell nature is also important for a design of molecular circuits by integrating single-molecule components.⁴ For example, the total current in the molecular circuit is affected by the spin polarization in the system. In this presentation, we illustrate the simulated difference in the *I-V* characteristics between the spin states of the diradical Ni₅ EMACs as shown Figure 1(a). After that, the electron conductivity of [18]annulene derivatives (Figure 1(b)) is focused on as a simplest example of the molecular parallel circuit to show a relationship between the diradical nature and quantum interference.

Keywords: electron conductivity, single-molecular device, molecular circuit, open-shell system

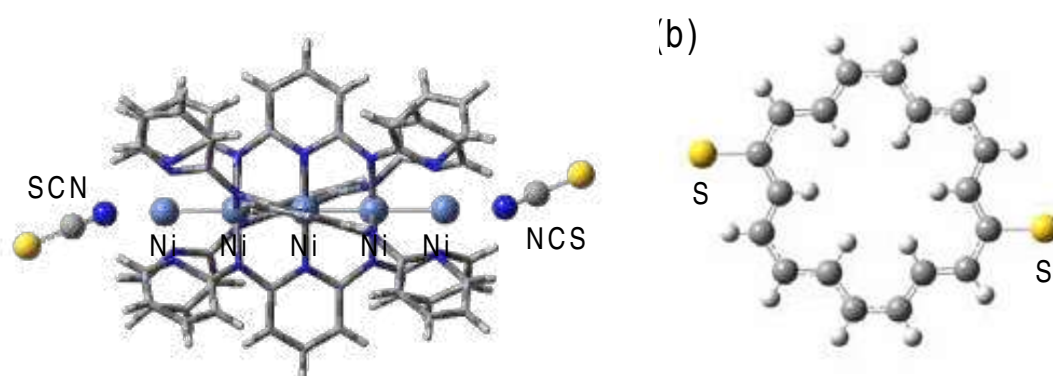


Figure 1. Molecular structures of (a) Ni₅ EMACs and (b) [18]annulene derivatives.

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DIRADICALOID Σ - AND Π -BONDS

Takashi Kubo^{a,b,c}

^a Graduate School of Science, Osaka University, Toyonaka, Osaka, Japan

^b Innovative Catalysis Science Division (ICS), Institute for Open and Transdisciplinary Research Initiatives (OTRI), Osaka University

^c Spintronics Research Network Division, Institute for OTRI, Osaka University.

*Corresponding author: kubo@chem.sci.osaka-u.ac.jp

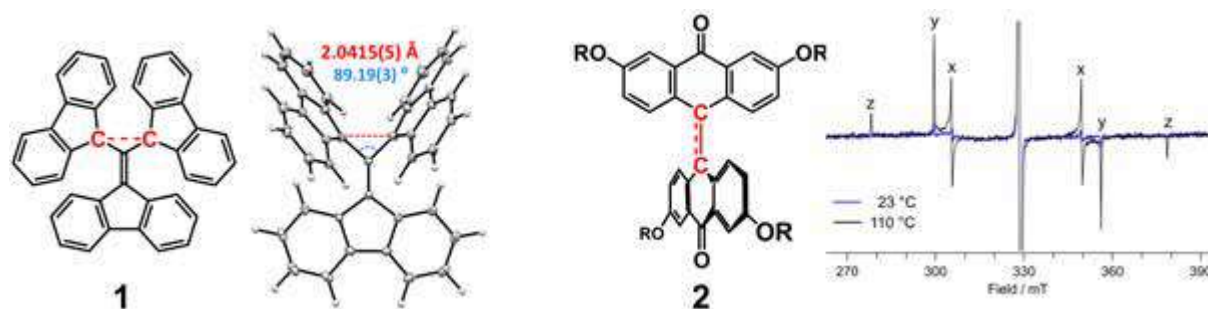
Abstract

The covalent bond is one of the most fundamental concepts in organic chemistry, wherein the strength of a covalent bond depends on the extent of the overlap integral between the orbitals of the atoms sharing the pair of electrons. The deviation from standard structures caused by the stretching, twisting, or bending of bonds leads to a reduction in the overlap of orbitals between atoms, and so the question of whether atoms in a special state are bonded or not is an important issue when defining covalent bonds. More specifically, σ -bond elongation and π -bond twisting have played an important role in learning the limits of covalent bonds.

In this presentation, I report the investigation of C–C bonding longer than 2.0 Å, which can be realized by perpendicularly facing two fluorenyl rings in the title compound **1**. A small orbital overlap between the distantly positioned carbon atoms was observed as a small concentration of electrons on the X-ray electron density map. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of the compound originated from the in-phase and out-of-phase interactions of the overlapping orbitals, respectively, with a gap of 2.39 eV. Solid-state ¹³C NMR spectroscopy showed a sharp peak at 82.9 ppm for the long-bonded carbons, and a CASSCF(6,6) calculation indicated small diradical character. The experimental and theoretical analyses revealed sufficient covalent bonding interaction in the long-bonded carbon pair.

I also focus on the covalent bonding character of a highly twisted double bond. Tetraoctyloxy bianthrone **2** was prepared and found to adopt a twisted conformation with the dihedral angle of 57°. The single crystal of **2** showed an ESR signal characteristic of a triplet species. From the variable temperature ESR measurements, the singlet–triplet energy gap was determined to be 24 kJ/mol, with the preference of the singlet state.

Keywords: Diradicaloid, Long single bond, Twisted double bond, Covalent bond, ESR



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STABLE POLYCYCLIC HYDROCARBON RADICALS AND DIRADICALS FROM A POP STRATEGY

Zhe Sun^{a,*}

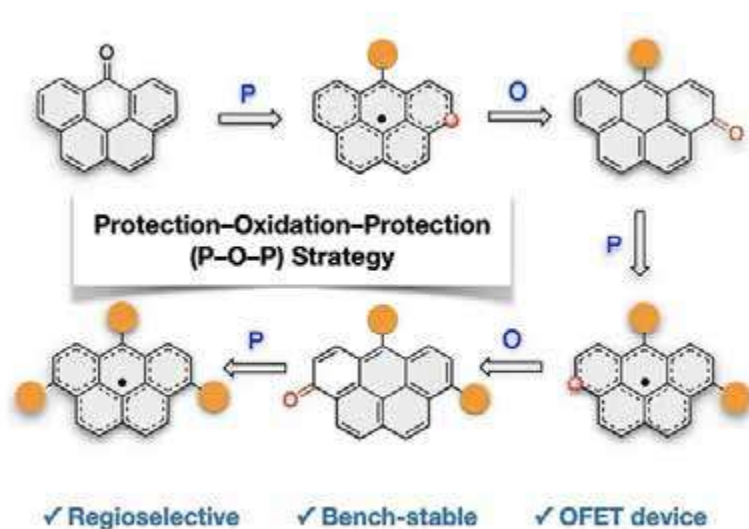
^aTianjin University

*Corresponding author: zhesun@tju.edu.cn

Abstract

Polycyclic hydrocarbon (PH) radicals are promising materials in the fields of organic (semi)conductors and biomedicines, but their practical applications are severely hampered by the challenging synthesis and insufficient stability. Here we introduce a protection-oxidation-protection (POP) strategy, in which substituents with various electronic and steric features can be introduced to the radical species. This POP strategy results in bench-stable organic radicals¹ and diradicals² (including non-Kekulé diradicals), and many of their properties, such as crystal packing, can be finely tuned. Consequently, we demonstrate that these open-shell materials are applicable in various fields, such as in field-effect transistors with excellent device stability in air, as well as in biological applications.

Keywords: polycyclic hydrocarbon, radical, stability, semiconductor, biomedicine



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PHOTOREACTIVITY AND PHOTODYNAMIC BEHAVIOR OF POLYCYCLIC AZIDES

Gudmundsdottir, Anna D.*^A

^AUniversity of Cincinnati

*Corresponding author: anna.gudmundsdottir@uc.edu

Abstract

Bendable crystals hold potential for use in flexible electronics, sensors, and actuators, where both flexibility and ordered structure are key for optimal performance. However, accurately predicting which organic crystals will bend upon exposure to light remains challenging. To explore this, we have been investigating organic azido crystals, as the irradiation of azido compounds releases N₂ gas,¹ which can trigger a photodynamic response, such as bending. Several examples of photo-bendable azido compounds will be presented, including polyaromatic-azides, demonstrating how their photodynamic behavior is governed by their crystal packing arrangements and photoreactivity. Specifically, we will present how the strength of intermolecular interactions between molecular layers influence their bendability, allowing the crystal to bend while maintaining the structure intact. A comparison between mechanical and light-driven bending will be discussed. In addition, we will present the influence of curvature on the physical properties and reactivity of corannulene nitrene in solution and cryogenic matrices, and compare its unique properties with those of flat polycyclic nitrenes.²

Keywords: Photodynamic Crystals, Corannulene Nitrene, Bendable Crystals

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LUMINESCENCE OF ASSEMBLED RADICALS

Tetsuro Kusamoto^{abc}

^aDepartment of Materials Engineering Science, Graduate School of Engineering Science, Osaka University

^bJST FOREST

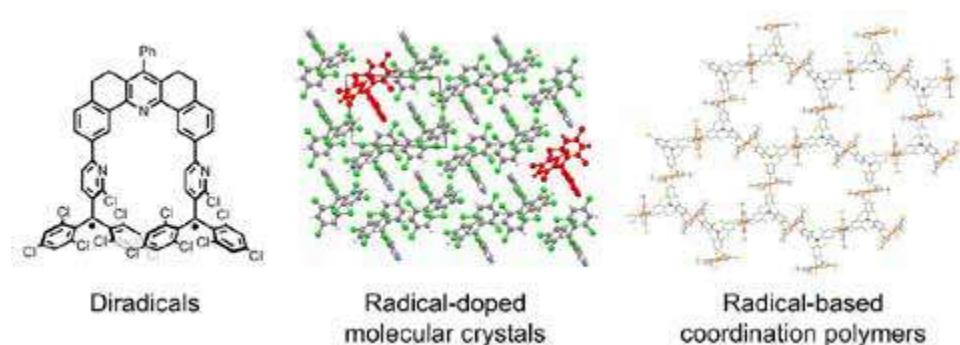
^cOTRI-Spin, Osaka Univ.

*Corresponding author: kusamoto.tetsuro.es@osaka-u.ac.jp

Abstract

Radicals can exhibit photofunctions unique to their open-shell electronic states, such as efficient electroluminescence, spin-allowed doublet-singlet and doublet-triplet energy transfer, and the absence of heavy atom effect.¹ These characteristics distinguish radicals from conventional closed-shell molecules and make them a new class of molecular emitters.²⁻⁷ We have shown that novel spin-correlated photofunctions, such as magnetic-field-controlled luminescence, emerge when radicals are assembled to interact with each other. This presentation highlights the spin-correlated luminescence of diradicals, radical-doped molecular crystals, and radical-based coordination polymers, emphasizing the uniqueness of the mechanism.

Keywords: luminescence, spin state, magnetic field effect



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CONTROLLING THE SINGLET–TRIPLET ENERGY GAP OF *m*-QUINODIMETHANE-BASED POLYCYCLIC DIRADICALS

Akihiro Shimizu,* Shinobu Arikawa, Tetsuya Morikoshi, Ryo Shintani*

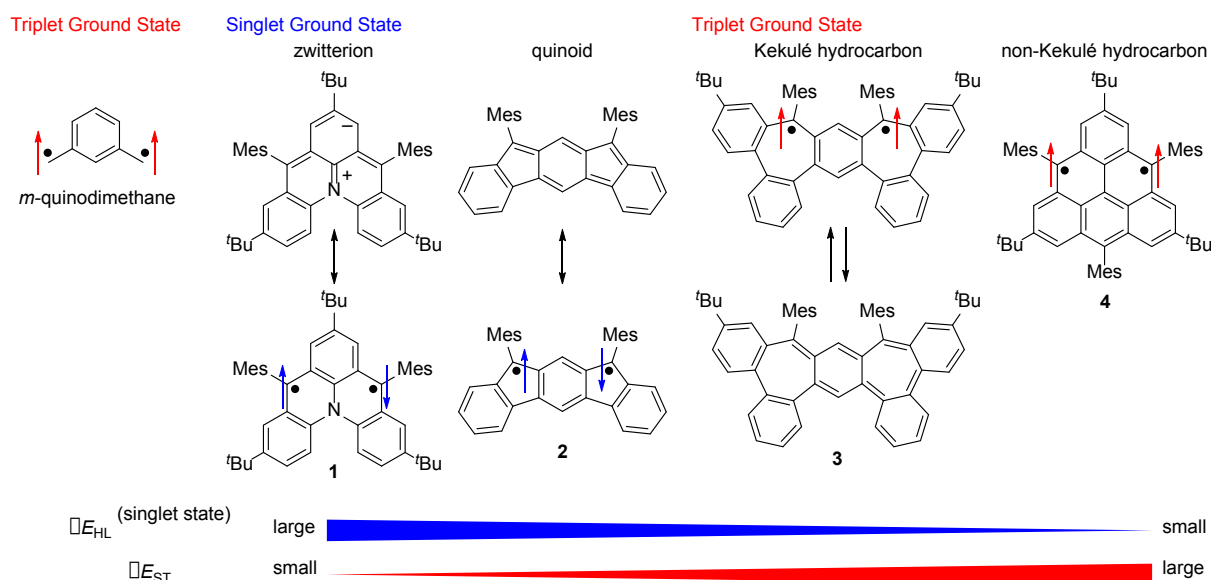
Graduate School of Engineering Science, Osaka University, Japan

*Corresponding authors: shimizu.akihiro.es@osaka-u.ac.jp, shintani.ryo.es@osaka-u.ac.jp

Abstract

Organic diradicals have long been studied as candidates for functional materials due to their unique electronic structure and optical, electrochemical, and magnetic properties derived from two unpaired electrons.¹ We have recently succeeded in the synthesis and isolation of *m*-quinodimethane-based polycyclic diradicals: zwitterionic open-shell singlet diradical **1**,² quinoidal open-shell singlet diradical **2**,³ Kekulé triplet diradical **3**,⁴ and non-Kekulé triplet diradical **4**.⁵ These diradicals show characteristic optical, electrochemical, and magnetic properties, such as near-infrared absorption, amphoteric redox properties, and strong ferromagnetic interaction. We clarified that there is a strong correlation between HOMO–LUMO energy gaps (ΔE_{HL}) and singlet–triplet energy gaps (ΔE_{ST}), indicating that diradicals with different spin multiplicity would be designed by controlling the interaction of unpaired electrons of *m*-quinodimethane.

Keywords: diradicals, singlet, triplet, quinodimethane, magnetic interactions



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STABLE AND ISOLABLE DIRADICALS WITH OLIGO(9,10-ANTHRYLENE)S

Yusuke Ishigaki*

Department of Chemistry, Faculty of Science, Hokkaido University, Japan

*Corresponding author: yishigaki@sci.hokudai.ac.jp

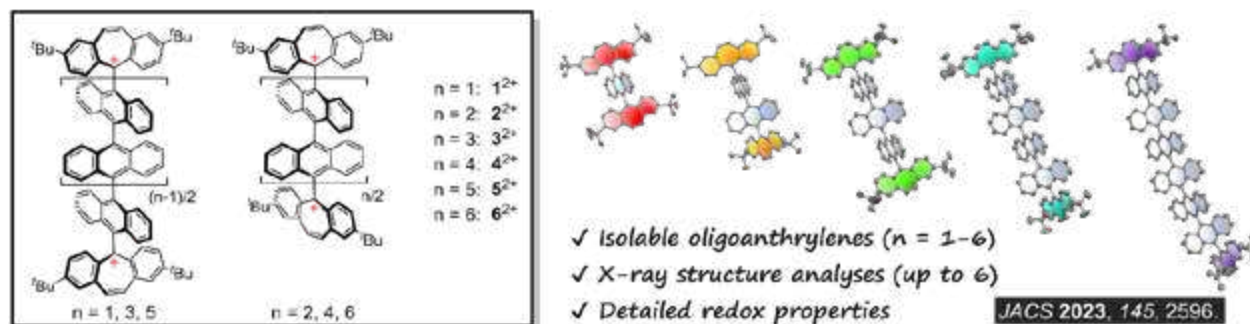
Abstract

Anthracene is a highly attractive 14π -aromatic unit due to its intriguing photophysical and electrochemical properties. Since anthracene can also be a key building block for a variety of organic molecules, oligoanthrylenes [X-(C₁₄H₈)_m-Y] have been reported thus far. Compared to the plethora of studies on 9,9'-bianthracene ($m = 2$) and its derivatives, there have been only a few reported examples of oligo(9,10-anthrylene) derivatives of $m \geq 3$, in which anthracene units are connected at 9,10-positions in a linear manner. Furthermore, there are no reports in which the geometrical features of oligo(9,10-anthrylene)s ($m > 3$) have been determined by X-ray analyses.

Herein, we designed a series of dications composed of pure hydrocarbons with one to six non-substituted 9,10-anthrylene units end-capped with two dibenzotropyliums. The six dication salts were synthesized from the corresponding diols, and their structures were successfully determined by X-ray analyses even in the case of eight consecutive 14π -aromatic units, revealing that all dications adopt almost orthogonally twisted structures between neighboring units. Therefore, the “cation-capping approach” could be a versatile strategy for overcoming the solubility problem and constructing unique response systems based on a large π -skeleton.^{1,2}

Spectroscopic and voltammetric analyses show that neither the significant overlap of orbitals nor the delocalization of electrons between 14π -electron units occurs due to the orthogonally twisted geometry even in solution. As a result, sequential oxidation processes were observed with the reversible formation of multivalent cations with the release of the same number of electrons as the number of anthrylene units. Furthermore, two-electron reduction of these dications can provide different types of molecular switches depending on the number of anthrylene units. For example, diradicals with more than two anthrylene units can be isolated as stable entities.

Keywords: cation-capping, cyclic voltammetry, molecular switch, redox system



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ELUCIDATION OF SPIN-CORRELATED LUMINESCENCE OF A CARBAZOLE-CONTAINING DIRADICAL EMITTER UNDER HIGH MAGNETIC FIELDS

Asato Mizuno

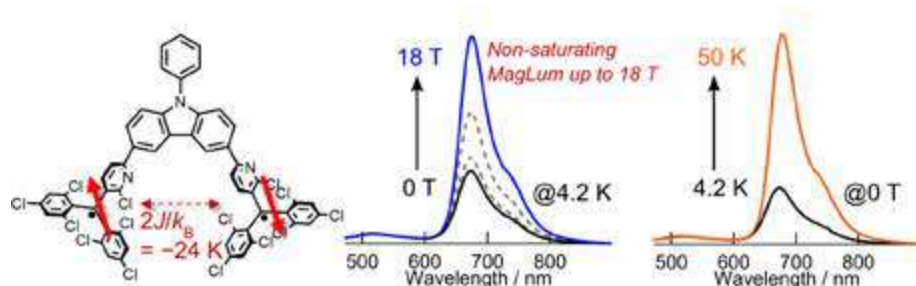
Department of Materials Engineering Science, Osaka University

*Corresponding author: mizuno.asato.es@osaka-u.ac.jp

Abstract

Luminescent radicals have been widely studied as a new class of materials exhibiting novel photofunctions unique to open-shell systems.^{1,2} Recent studies on luminescent diradicals have revealed intriguing spin-dependent emission (or spin-correlated luminescence), which can be modulated by magnetic field and/or heat.^{3,4} In this presentation, detailed mechanisms of the spin-correlated luminescence, which are revealed by luminescence measurements of a carbazole-containing diradical emitter under high magnetic fields, will be presented.⁵

Keywords: luminescence, high magnetic fields, diradical



- ✓ Ground-state-dominated **MagLum** and **thermally-activated emission**
- ✓ Photoluminescence quantum yields of up to 0.28 in solution
- ✓ External heavy-atom effect on luminescence

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OPEN-SHELL GRAPHENE FRAGMENTS AS SYNTHONS OF CARBON NANOSTRUCTURES

Michal Juriček*

Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

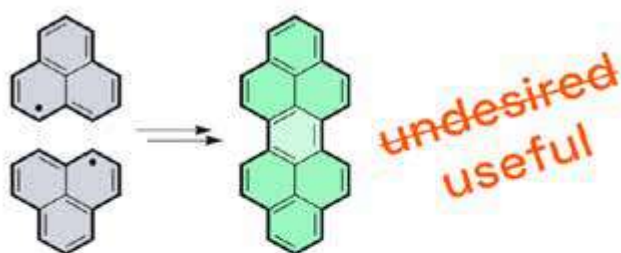
*Corresponding author: michal.juricek@chem.uzh.ch

Abstract

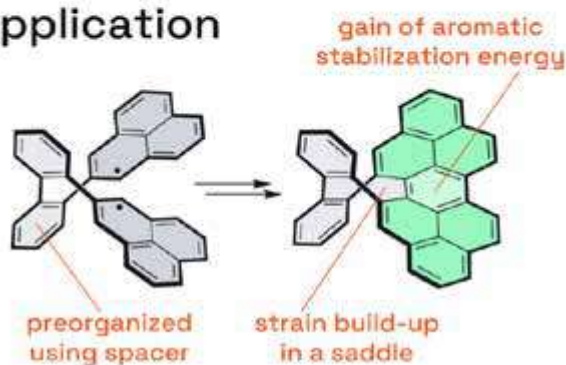
Open-shell graphene fragments are envisioned as promising future materials, in which spin interactions between unpaired electrons enable control of quantum information or induce magnetism, features sought-after in spintronics and quantum molecular science. Our research team designs and develops methods to make synthetic nanographene π -radicals and explore the fundamental aspects of their properties, by utilizing the presence of unpaired electrons to create function. While the reactivity of these systems is traditionally viewed as a limitation, we have uncovered specific, well-defined reaction pathways in π -radicals that open new avenues for designing complex graphene-based nanostructures. This shift in perspective has led us to harness reactivity as a synthetic tool, guiding us to develop precise strategies to modulate and control these reactions. In this presentation, we will share our recent progress in implementing this concept, including key examples from our latest work^[1–4].

Keywords: π -radical reactivity, open-shell polycyclic hydrocarbon, phenalenyl, triangulene

Concept



Application



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LEWIS ACID COUPLED ELECTRON TRANSFER AND DIRADICALS

Xinping Wang*

Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032

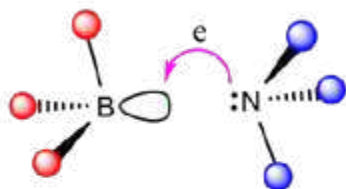
*Corresponding author: xpwang@sioc.ac.cn

Abstract

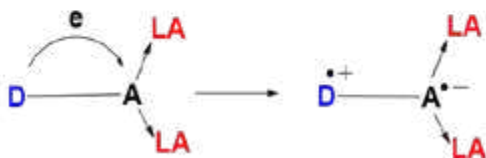
Single electron transfer (SET) exists widely in chemical, biological and material systems. Proton coupled electron transfer (PCET) is a typical example. In 2013, we observed that Lewis acid $B(C_6F_5)_3$ (BCF) oxidized an organic molecule by single electron transfer. Since then, single-electron oxidizing organic molecules by classic Lewis acids have been extensively studied. In recent years, we have focused on the development of Lewis acid coupled electron transfer (LACET) using BCF and other classic Lewis acids, and studied its application in various fields. In this talk, we will present a new class of diradicals formed by LACET strategy.

Keywords: Lewis acid, electron transfer, diradical

a) Single electron transfer between a Lewis acid and base



b) Lewis acid-coupled single electron transfer (LACET)



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LIGHT EMISSION IN DIRADICALS AND TRIRADICALS

Juan Casado^{a,*}

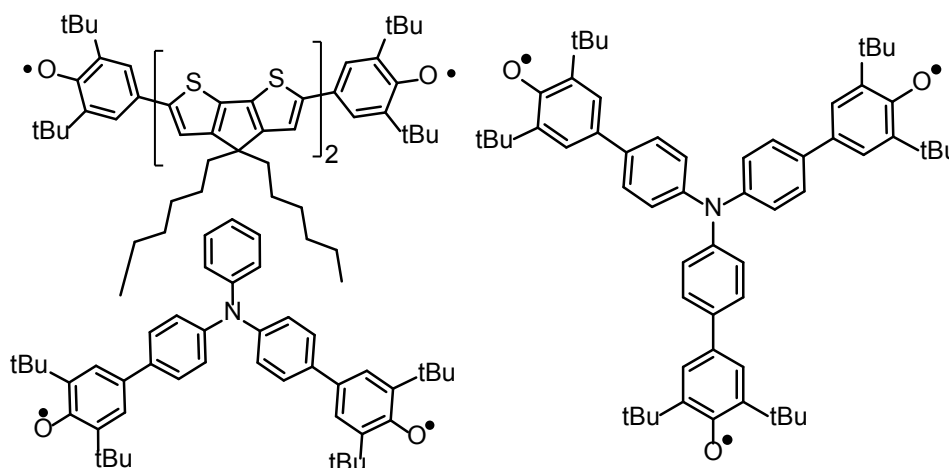
^aDepartment of Physical Chemistry, Faculty of Science, University of Málaga,
Campus de Teatinos, s/n 29071 Málaga, Spain.

*Corresponding author: casado@uma.es

Abstract

Diradicals or diradicaloids are characterized by low energy absorptions as a result of the weak bonding coupling between the unpaired electrons. Narrow optical gaps are detrimental for light emission given the extreme efficiency of non-radiative mechanisms including electron transfer and intersystem crossing.¹ Recently, however, monoradicals² have been shown to disclose doublet fluorescence with optical gaps in the visible region and approaching the near-infrared spectral region. The combination of magnetism (unpaired electrons) and light emission are great ingredients to achieve more versatile functional materials. Herein, we show light emission in a diradical molecule based on end-capped bis(benzoquinone) quinoidal oligothiophenes³ (Figure 1) with medium diradical character and showing light emission well penetrating in the NIR spectra region, at 1100 nm, as a result of the fine balance between the low energy lying ionic excited states. In addition, a comparative study of galvinoxyl-based radical, diradical and triradical (Figure 1) will be also presented and analyzed/discussed from the point of view of their emission properties.⁴

Keywords: fluorescence, diradical, triradical, benzoquinone, galvinoxyl



Graphic 1. Chemical structures of the studied compounds

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4. Manuscript in preparation.

LOW-COORDINATED GERMANIUM IN THE RING: UNUSUAL STRUCTURES AND REACTIVITY

Yoshiyuki Mizuhata

Institute for Chemical Research, Kyoto University

**Corresponding author: mizu@boc.kuicr.kyoto-u.ac.jp*

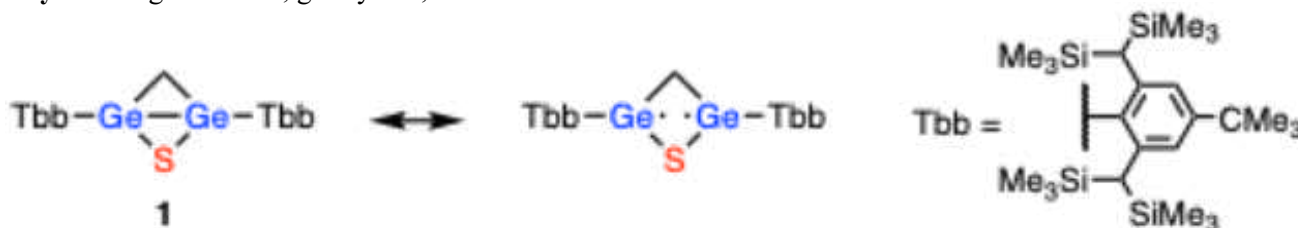
Abstract

Our research is aimed at elucidating the unique structures and reactivity exhibited by low-coordinated compounds of heavy main group elements and extracting their functions. In particular, we have been actively engaged in the creation of a variety of molecules incorporating low-coordinated group 14 elements into ring structures. Recently, we have developed the chemistry of “heavy phenyl anions”, in which the anionic carbon of the phenyl anion is replaced by germanium or tin,¹⁻⁴ for application in atomic germanium transfer reactions.⁵

More recently, we have found methylene-bridged bis(germylene) to be useful in the synthesis of a variety of compounds with novel bonding modes. In particular, we found *in-situ* formation of 2-thia-1,3-digermbicyclo[1.1.0]butane **1**, a heavy element analogue of 2-oxabicyclo[1.1.0]butane,⁶ one of the unexplored molecules. Reflecting its diradical nature, **1** is a highly reactive compound that undergoes an addition reaction to the solvent benzene. Interestingly, heating the C₆D₆ solution of the benzene-adduct resulted in the exchange of C₆H₆ moiety to C₆D₆. This indicates that benzene-adduct can be used as a precursor for the generation of **1**.

In this presentation, the structure and properties of compounds obtained by the reactions of bis(germylene) will be reported, as well as details of the properties of **1**.

Keywords: germanium, germylene, benzene activation



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SUSTAINABLE PREPARATION OF WHO ESSENTIAL MEDICINES BY MECHANOCHEMISTRY

Evelina Colacino*

ICGM, Univ Montpellier, CNRS, ENSCM, 34293 Montpellier, France.

*Corresponding author: evelina.colacino@umontpellier.fr

Abstract

Although there have been efforts to reduce the environmental impact of active pharmaceutical ingredient (API) production, the use of organic solvents (responsible for 75% of energy used) is still a critical step in many processes. Solvent-free (or low solvent) synthesis by mechanochemistry^{1,2} fulfils several of the 12 Green Chemistry Principles³ and it is a promising sustainable and enabling technology to prepare value-added chemicals and pharmaceutically relevant fragments and functionalities, including APIs.

This presentation highlights case studies for preparing World Health Organization (WHO) essential medicines by mechanochemical processes, at different scales. The assessment by green chemistry metrics⁴ showcases how mechanochemistry can offer an eco-friendly and cost-effective pathway also to green pharmaceuticals, contributing in perspective, ‘to make our planet more sustainable’.⁵

Keywords: Mechanochemistry, Active Pharmaceutical Ingredients, Rearrangements, Green metrics.

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ORGANIC MECHANOCHEMISTRY – PAST, PRESENT AND FUTURE

Davor Margetić^{a,*}

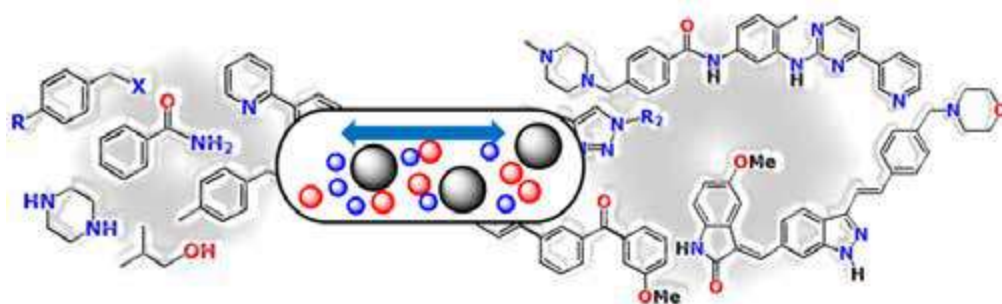
^a Laboratory for Physical-Organic Chemistry, Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička c. 54, 10000 Zagreb, Croatia

*Corresponding author: margetid@irb.hr

Abstract

The global need for a transition toward more environmentally green and sustainable chemical processes led to the development of diverse approaches and methodologies.¹ Mechanochemistry, a nonconventional method where the chemical reaction is induced by applying mechanical energy in the solid state holds some sustainability advantages for synthetic manufacturing processes. This synthetic methodology allows the simple, rapid, and clean synthesis of molecules by more efficient use of resources, minimizing energy consumption, and reducing waste production. The high potential of mechanosynthesis is recognized by the IUPAC as one of the emerging technologies for a more sustainable future and it is nowadays a fast-developing area for various applications in the production of organic chemicals and materials.²⁻⁸ The historical and current overview of this environmentally greener method and its applications in preparing various organic compounds and materials will be presented.

Keywords: mechanochemistry, organic synthesis, solid-state reactions, green chemistry, sustainability



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MECHANOCHEMISTRY FOR REVOLUTIONARY EFFICIENT SYNTHESIS ORGANIC AND ORGANOMETALLIC COMPOUND

Hajime Ito

Division of Applied Chemistry and Frontier Chemistry Center, Faculty of Engineering, and Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Hokkaido, Japan.

**Corresponding author: insert email address*

Abstract

Mechanochemical synthesis, which utilizes little amount of or no solvent, provides a sustainable alternative to conventional solution-based organic synthesis. By replacing solvents and standard glassware with ball mills, this method not only minimizes solvent use but also introduces several compelling advantages: accelerated reaction rates due to high-concentration conditions, compatibility with insoluble compounds, activation of substrates via mechanical forces, and improved selectivity and yield. Leveraging these benefits, we have successfully demonstrated various applications, including Suzuki coupling with insoluble compounds,^{1,2} “mechanoredox” reactions using piezoelectric materials,³ synthesis of organometallic compounds such as Grignard reagents via ball milling,⁴ and “ultra-fast” one-minute Birch reduction.^{5,6} This talk will highlight our latest research on mechanochemical synthesis, showcasing its transformative potential in advancing organic synthesis.

Keywords: mechanochemistry, cross-coupling, piezoelectric, Grignard reaction, Birch reduction

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REACTION PATHS IN ORGANIC MECHANOCHEMISTRY BY IN-SITU MONITORING

Ivan Halasz^{a,*}

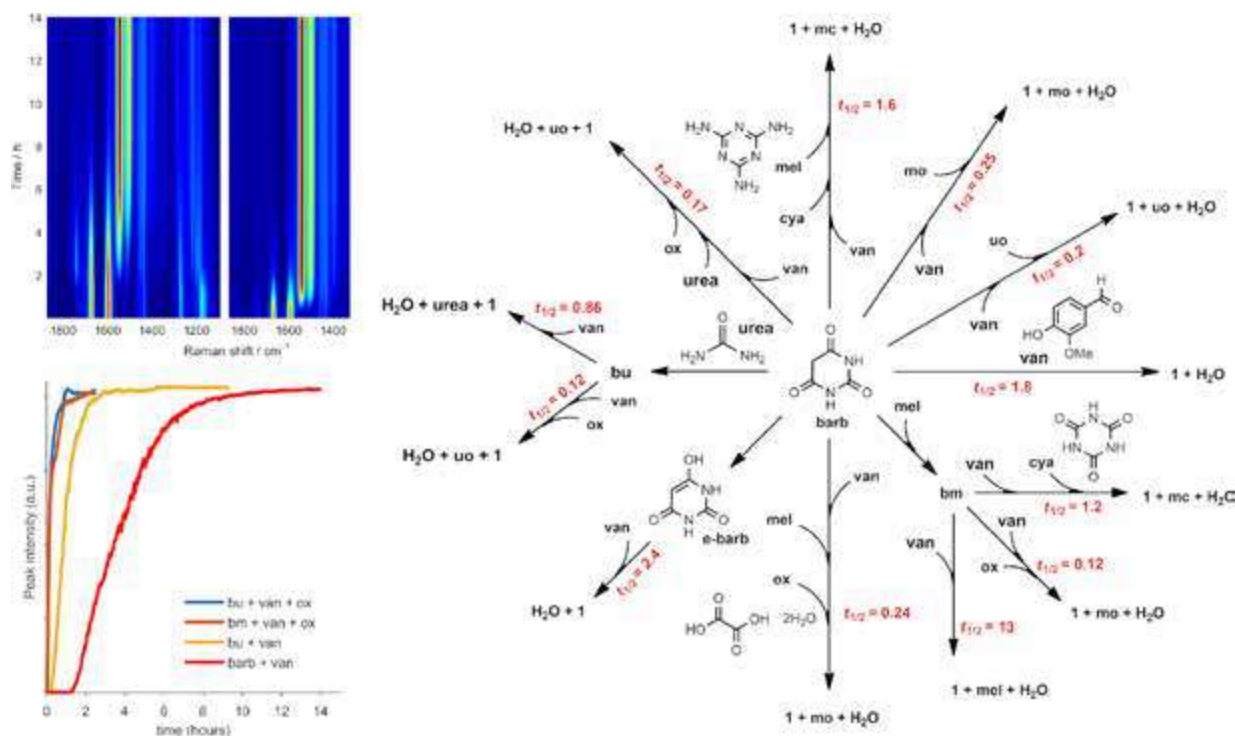
^aRuder Bošković Institute, Zagreb, Croatia

*Corresponding author: ihalasz@irb.hr

Abstract

Recent advancements in real-time monitoring techniques have transformed our comprehension of mechanochemical reactions, which were previously difficult to study due to their occurrence in sealed, opaque containers.¹ These innovative methods enable continuous observation of milling processes without disrupting the reaction or exposing the contents. They unveil a dynamic reaction environment that is highly sensitive to minor changes in conditions. Our research using in-situ Raman spectroscopy has illuminated reaction mechanisms, intermediates, and kinetics. We've also demonstrated the occurrence of atomic and molecular exchanges during mechanochemical processes. Furthermore, we've shown how altering the solid forms of reactants can influence specific reaction pathways and rates.² Our work underscores the benefits of solid-state mechanochemistry compared to conventional solution-based methods, not only in terms of cleaner and more sustainable synthesis, but also in achieving product selectivity that may be challenging to attain in solvent-based chemistry.

Keywords: Mechanochemistry, Raman in situ monitoring, solid forms, reaction mechanism, kinetics



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RECENT ADVANCES IN MECHANOCHEMICAL ORGANIC REACTIONS

Guan-Wu Wang^{a,b*}

^a School of Chemistry and Materials Science, Anhui Normal University, Wuhu, Anhui 241002, P. R. China

^b Department of Chemistry, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China

*Corresponding author: gwang@ustc.edu.cn; gwang@ahnu.edu.cn

Abstract

Over the years, mechanochemical organic synthesis has garnered increasing attention due to its unique advantages. These reactions are typically conducted in ball mills under solvent-free conditions or via liquid-assisted grinding (LAG), offering benefits such as high reaction efficiency, precise stoichiometric control, and reduced waste generation compared to traditional solvent-based methods.^{1,2} In this talk, I will highlight our recent advances in the mechanochemistry of fullerene and non-fullerene molecules, showcasing their potential in sustainable synthetic strategies.

Keywords: mechanochemistry, fullerenes, non-fullerene molecules, solvent-free, green organic synthesis

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ARE PLASTIC WONDER MATERIALS OR A CURSE ON ECOLOGY AND HUMAN LIFE?

Suresh Valiyaveetil

Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117548

**Corresponding author: chmsv@nus.edu.sg*

Abstract

Plastic materials made from a wide range of polymers are used in almost every aspect of our day-to-day life. However, the linear synthetic strategy used for preparing common polymers only involves ease of production, high stability and processability with no circularity or sustainability. Large amounts of different polymers are produced and processed annually, but used polymer-based objects are difficult to recycle or reuse for multiple practical reasons. As a result, significant amounts of used plastic materials end up in the environment. Such plastic wastes in the environment undergo slow degradation and release small particles called micro- and nanoplastic particles. Even though, many studies pointed out the toxicity of additive chemicals such as phthalates and bisphenol A, present in plastics, only limited knowledge exists on the adverse impact of plastic particles on the health of terrestrial or aquatic animals. To address the plastic waste issues, a few groups are working on developing sustainable polymers to replace synthetic ones. We focus on understanding the biological impact of plastic particles using animal and human cellular models. Our results indicate that toxicity or adverse health impact of the nanoparticles of common polymers depends on the choice of animal models and the chemical nature of the polymers used. In a comparative study, fluorescent polymethylmethacrylate (PMMA), and polyvinylchloride (PVC) nanoparticles were used to explore the uptake, translocation, and toxicity in various biological models. PVC nanoparticles caused high mortalities in different animal and cellular models. The talk will provide some of our recent results and challenges in this area.

FUNCTIONAL POLYMERS: FROM NEW SYNTHETIC ROUTES TO APPLICATIONS IN ENERGY STORAGE

Patrick Théato^{a,b*},

^a*Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology (KIT), Engesser Str. 18, D-76131 Karlsruhe, Germany.*

^b*Soft Matter Synthesis Laboratory, Institute for Biological Interfaces III, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany.*

**Corresponding author: patrick.theato@kit.edu*

Abstract

Functional polymers are based on certain chemical functional groups. As such, the inspiration from organic chemistry has always been fruitful to the development of new synthetic routes to functional polymers. Further, the thrive for structure-property relationships in polymer materials requires a precise control of polymer structures. As such, two different aspects will be discussed:

Poly(ethylene oxide) PEO is a readily investigated polymer in numerous applications. One of them being its utilization as an electrolyte for solid-state batteries. However, not much is known on structural variants of PEO about the utilization as polymer electrolytes. Herein, we present the synthesis of some novel PEO-based polymer architectures and their utilization as polymer electrolytes.

Sulfur and particular functional groups derived from sulfur have been major players in this area of exciting research and further have been utilized for the design and preparation of polymeric materials that lead to a plethora of applications. Sulfur as a side product of natural gas and oil refining is an underused resource. Converting landfilled sulfur waste into materials merges the ecological imperative of resource efficiency with economic considerations. A strategy to convert sulfur into polymeric materials is the inverse vulcanization reaction of sulfur with alkenes. However, the materials formed are of limited applicability, because they need to be cured at high temperatures (>130 °C) for many hours. Herein, we discuss the reaction of elemental sulfur with vinyl alkoxysilanes to enable a control of materials properties. Also, post-polymerization modifications of such inverse vulcanized polymers will be discussed.

Keywords: Energy Storage, PEO polymer, inverse vulcanization, post-polymerization modification, flow chemistry

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TOWARD 3-DIMENSIONAL ORGANIC MIXED IONIC-ELECTRONIC CONDUCTOR STRUCTURES

Myung-Han Yoon^{a*}

^a*Department of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST),
Republic of Korea*

^{*}*Corresponding author: mhyoon@gist.ac.kr*

Abstract

In this research, we report organic bioelectronic interfaces based on highly crystalline organic mixed ionic-electronic conductors (OMIECs) to overcome the trade-off between electrical/electrochemical performance and long-term stability in water. First, by introducing sulfuric acid treatment, we crystallized poly(3,4-ethylenedioxythiophene):poly styrene sulfonate (PEDOT:PSS) films which exhibit excellent electrical/electrochemical/optical properties, long-term aqueous stability, and good biocompatibility for primarily cultured cardiomyocytes and neurons over several weeks. Furthermore, they are successfully employed for high-performance multi-electrode arrays to record and stimulate the electrophysiological activities of primarily cultured cardiomyocytes and chicken retinae tissues. Next, crystalline PEDOT:PSS microfibers and their self-fusion process are developed for single-strand wearable electrochemical transistors and 3D microfibrillar network-based bioelectronic interfaces. Finally, direct crystallization of PEDOT:PSS on plastic substrates, carbon nanotube yarn/PEDOT:PSS core-shell fibers for energy storage devices, PEDOT:PSS/Pt nanoparticles composite materials for electrocatalysis and gas separation, and PEDOT:PSS/clay composite-based biodegradable/sustainable electronics are briefly discussed.

Keywords: organic mixed ionic-electronic conductors, PEDOT:PSS, bioelectronics

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ALGINATE-BASED MICROSPHERES FOR ENCAPSULATION OF PANCREATIC ISLETS IN DIABETES TREATMENT

Igor Lacík^{a,*}

^a*Polymer Institute of the Slovak Academy of Sciences, Bratislava, Slovakia*

**Corresponding author: igor.lacik@savba.sk*

Abstract

Currently available insulins, glucose sensing and insulin administration technologies offer increasingly accurate control of blood glucose levels in diabetes treatment. However, a significant number of diabetic patients are unable to maintain physiological glucose levels that results in health complications [1]. For such group of patients, the transplantation of functional pancreatic islets represents a solution [2]. In the case of allogeneic transplants, immunosuppression is necessary to protect the islets from the body's immune reaction.

The objective of this work is to develop polymeric microspheres that are suitable for long-term immunoprotection of transplanted islets. At the same time, microspheres ensure the long-term survival and functioning of the islets, i.e., insulin production based on the immediate glucose levels. Alginate-based microspheres have been proposed as a suitable encapsulation material and tested in animal models as well as in clinical trials [3]. These microspheres are stabilized either by divalent cations or by polyelectrolyte complexation, or both.

The encapsulation community strives for recognizing the factors that are important for the survival and function of encapsulated islets in animal models with the vision of clinical trials. In this contribution, the factors important for biocompatibility and stability in designing alginate microbeads [4] as well as multicomponent alginate-based polyelectrolyte microcapsules [5] will be discussed from synthesis and characterization of polymers, process of encapsulation, physical, chemical, and biological characterization of microspheres, to animal experiments.

The significance of working on this topic is the clinical option affording the control of the blood glucose levels by transplanted islets without the need for immunosuppression. Such principle can be used for immunoprotection of transplanted cells also in other cell therapies.

Keywords: diabetes treatment, transplantation of encapsulated islets, alginate, microspheres, polyelectrolytes

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TOWARDS CIRCULAR HIGH-PERFORMANCE COMPOSITES VIA CHEMISTRY

William E. Dyer^a, Dimitrios Apostolidis^a, Niklas Lorenz^a, Baris Kumru^{a*}

^a*Aerospace Structures & Materials Department, Faculty of Aerospace Engineering, Delft University of Technology, 2629 HS Delft, The Netherlands*

^{*}*Corresponding author: b.kumru@tudelft.nl*

Abstract

Advances in chemistry have revolutionized materials engineering, enabling the development of lightweight carbon fiber-reinforced polymer composites (CFRP) that now comprise over 50% of the structural weight in modern aircraft. Compared to traditional metals and alloys, CFRPs have significantly reduced weight, improved fuel efficiency, lowered costs, and made aviation more accessible as a public transportation option.¹ However, the widespread use of thermosetting polymer matrices, particularly epoxy resins, poses significant challenges due to their lack of recyclability and reliance on fossil-derived feedstocks.²

To transition toward a circular composites industry, a stronger integration of chemistry and engineering is essential. This requires exploring renewable feedstocks for high-performance resin formulations while assessing their manufacturing and engineering viability through standardized mechanical tests (e.g., ASTM) which is currently missing in literature.³

In this presentation, I will highlight our recent advancements in chemical technologies tailored for aerospace applications. These include the development and evaluation of renewable, high-performance epoxy resin systems and step by step guide on formulation and analysis will be presented.⁴ Additionally, epoxy-based vitrimeric resins that enable reparability and recyclability in composites will be explained.⁵ By leveraging chemical technology, we aim to address the sustainability challenges of CFRP and pave the way for a more circular and sustainable composites industry.

Keywords: resin engineering, circular composites, polymer composites, renewable resin, applied chemistry



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STRUCTURES AND PROPERTIES OF CATECHOL-MODIFIED HYDROGELS

Jungju Ryu^a, Minjeong Kang^a, Daewon Sohn^{a*}

^a Department of Chemistry and Research Institute for Convergence of Basic Science, Hanyang University, Seoul 04763, Korea.

*Corresponding author: dsohn@hanyang.ac.kr

Abstract

We developed hyaluronic acid (HA) hydrogels by regulating the gelation kinetics of Fe^{3+} and a catechol cross-linker, including Fe^{3+} -induced covalent bonding and coordination bonding. Dual roles of Fe^{3+} in catechol-modified HA (HA-CA), Fe^{3+} -catechol coordination, and catechol oxidation followed by a coupling reaction, were selectively applied for different gelations. Tetra-poly(ethylene glycol) with catechol end groups (t-PEG-CA) was also crosslinked through coordination bonds between catechol moieties and Fe(III) ions, which produce bis-complex and tris-complex depending on pH levels. This study investigated the property-structure relationship of crystalline polymer gels formed by coordination bonds, focusing on Fe(III) -catechol crosslinked tetra-arm polyethylene glycol (4-PCA) hydrogels. Thermo-rheological properties of gels were examined within the crystallization temperature range by differential scanning calorimetry (DSC) and rheometer. As the hydrogel was formed by bis coordination bonds at pH 8, the crystallization temperature was significantly lowered, which aligns with our hypothesis. At temperatures below 20°C and lower frequencies, the loss modulus (G'') of 4-PCA gels crossovers with the storage modulus (G'), indicating the gel point, but not above 30°C . The study demonstrates that at low temperatures, gels are formed through coordination bonds, resulting in a highly organized lamellar structure with relatively large periodic spacing between the layers. It indicates that the gel's unique structural properties are temperature-dependent and closely linked to the specific interactions occurring during gelation.

Keywords: hydrogel, hyaluronic acid, catechol, tetra-poly(ethylene glycol), gelation



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SYNTHESIS OF HIGH PERFORMANCE POLYMERS FROM NATURALLY OCCURRING MYO-INOSITOL

Atsushi Sudo^{a*}

^a Graduate School of Science and Engineering, Kindai University

*Corresponding author: asudo@emat.kindai.ac.jp

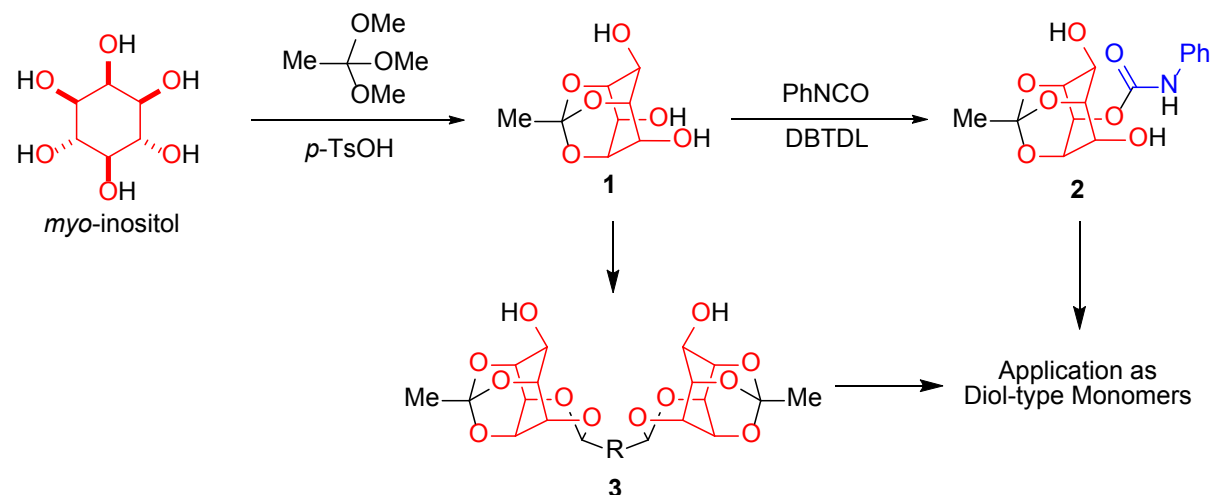
Abstract

Efforts to develop high-performing bio-based polymers have intensified, aiming to replace petroleum-based polymers with renewable alternatives for societal sustainability. Among various strategies, deriving rigid diols from naturally occurring compounds has shown promise in creating polymers such as polyesters, polycarbonates, and polyurethanes with high heat resistance. The rigid structures of these diols restrict polymer chain motion, increasing glass transition temperatures (T_g).

Our focus has been on *myo*-inositol, a renewable resource derived from nonedible bioresources such as rice bran and bean skin. Regioselective reactions of *myo*-inositol hydroxyl groups yield highly rigid derivatives, including cyclic acetals and orthoesters. Notably, orthoester **1**, a triol with an adamantane-like motif, serves as a precursor for rigid monomers. Its reaction with phenyl isocyanate produces a diol monomer **2**, which, upon polyaddition with hexamethylene diisocyanate (HMDI), forms polyurethanes with T_g values up to 105 °C, comparable to isosorbide-derived polyurethanes.

This study presents a novel design for diol monomers **3** synthesized from *myo*-inositol. The diol incorporates two orthoester moieties connected via acetalization, creating cyclic acetals to enhance rigidity. These structural features enable the synthesis of polymers with high adamantane-like content. Polyaddition with diisocyanates demonstrates the potential of diol **3** for producing high- T_g polymers, advancing the development of bio-based engineering materials.

Keywords: bio-based polymers, rigid diols, *myo*-inositol, high T_g polymers



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TADF EMITTER AND THEIR APPLICATION IN VACUUM-DEPOSITED OLEDs

Man-Chung Tang*, Cangyu Wang, Xiaoge Song and Si-Jie Li

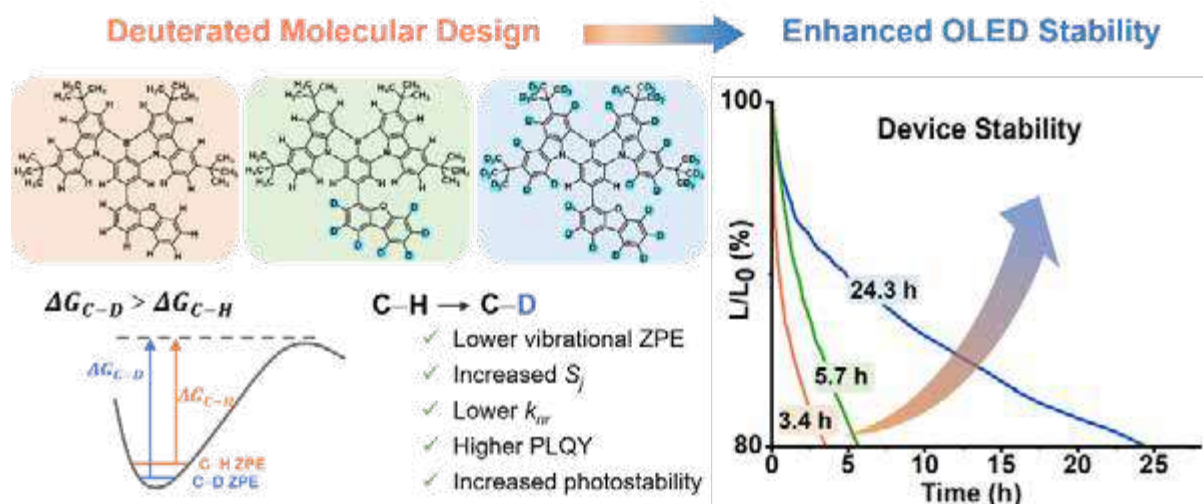
Institute of Materials Research, Tsinghua Shenzhen International Graduate School,
 Tsinghua University, Shenzhen 518055, China

*Corresponding author: kobetang2021@sz.tsinghua.edu.cn

Abstract

Multiple-resonance thermally activated delayed fluorescence (MR-TADF) emitters have garnered significant attention in recent years due to their remarkable properties, such as high luminescent quantum yield, robustness, and their compliance with the Broadcast Television 2020 standard for the new generation of ultrahigh-definition. Despite these advancements, the operational lifetimes of organic light-emitting diodes (OLEDs) relying on MR-TADF emitters still fall short of practical application. We believe that enhancing the intrinsic molecular stability of ¹Bu-DABNA, a fundamental backbone of MR-TADF emitters, holds great promise to be a universal strategy for all MR-TADF emitters, improving the operational lifetimes of OLEDs. Herein, we report the design and synthesis of targeted deuteration on the donor and/or backbone of MR-TADF emitters and investigate the hyperconjugation effect of Si- and Ge-containing auxiliary ligand MR-TADF emitters. We also examine the structure-property relationship between intrinsic molecular stability upon isotopic and hyperconjugation effects towards device operational stability.

Keywords: MR-TADF; OLED; Deuterated; Hyper-conjugation effect; Device Optimization



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LUMINESCENT ORGANOSILANE AND ORGANOGERMANE MR-TADF EMITTERS FOR OPERATIONALLY STABLE BLUE ORGANIC LIGHT-EMITTING DIODES

Si-Jie Li,^a Xiongkai Tang,^{a,b} Chiu Hwi Ng,^c Jia Yang Lim,^c Wai Kit Tang,^c Wen-Cheng Chen,^d Yanping Huo,^d Maggie Ng,^{a,*} Season Si Chen,^{*b} Dongdong Zhang,^c Lian Duan,^{c,f} Man-Chung Tang^{a,*}

^a*Institute of Materials Research, Tsinghua Shenzhen International Graduate School, Tsinghua University, Shenzhen, 518055, China*

^b*Institute of Environment and Ecology, Tsinghua Shenzhen International Graduate School, Tsinghua University, Shenzhen, 518005, China*

^c*Department of Chemistry, Faculty of Science, University of Malaya, Kuala Lumpur, 50603, Malaysia*

^d*School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou, 510006, China*

^e*Key Laboratory of Organic Optoelectronics and Molecular Engineering of Ministry of Education, Department of Chemistry, Tsinghua University, Beijing, 100084, China*

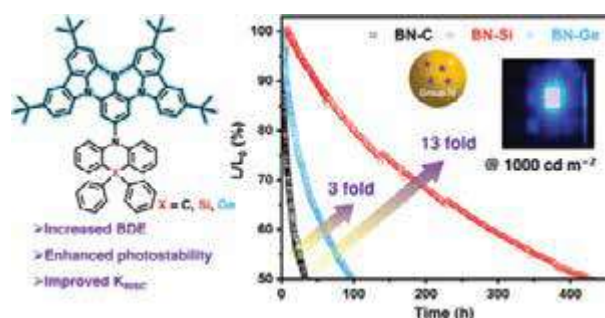
^f*Laboratory of Flexible Electronics Technology, Tsinghua University, Beijing, 100084, China*

*Corresponding author: maggie.ng.0121@connect.polyu.hk; season.chen@sz.tsinghua.edu.cn; kobetang2021@sz.tsinghua.edu.cn

Abstract

Organic light-emitting diodes (OLEDs) require highly stable blue emitters for long-term operational performance. In this study, we investigated the impact of incorporating silicon (Si) and germanium (Ge) into multiple-resonance thermally activated delayed fluorescence (MR-TADF) emitters to enhance luminescence efficiency and intrinsic stability. Theoretical calculations reveal that Si and Ge participate in conjugated systems via hyperconjugation effects, strengthening C–Si and C–Ge bonds and increasing bond dissociation energies (BDEs). These improvements lead to enhanced molecular photostability, as confirmed by density functional theory (DFT) and time-dependent DFT (TDDFT) calculations. Spin-orbital coupling (SOC) and spin-vibronic coupling (SVC) analyses indicate that flexible conformations facilitate efficient spin-flip processes, by enriching the characters and density of their excited states. Experimental validation through OLED fabrication demonstrates a maximum external quantum efficiency (EQE) of 30.0% for BN-Ge-based devices, with a CIE_y ≤ 0.18. The developed deuterated hole-transporting and host materials further improve operational stability, achieving LT₉₀ values of 48.3 and 7.1 hours for BN-Si and BN-Ge-based OLEDs, respectively. These findings provide a theoretical and experimental framework for the rational design of group IV element-containing MR-TADF emitters in next-generation optoelectronic applications.

Keywords: deuteration, MR-TADF, operational stability, organogermane, organosilane



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LARGE-AREA CRYSTALLINE CONJUGATED POLYMERS AND DEVICES

Huanli Dong^{a*}, Yumin Liu^a, Jingyue Yan^a, Mingxin Li^a

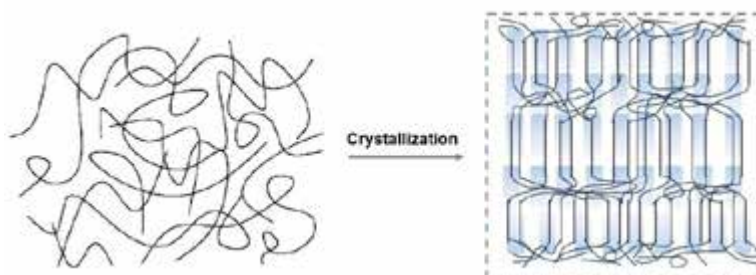
^aKey Laboratory of Organic Solids, Institute of Chemistry, The Chinese Academy of Sciences, Beijing 100190, China

*Corresponding author: dhl522@iccas.ac.cn

Abstract

Large-area conjugated polymers with high carrier mobility have been actively pursued for numerous applications, such as flexible circuits and wearable electronics¹. The carrier mobility is an important figure of merit that is sensitively influenced by the crystallinity and the molecular arrangement. One key challenge with conjugated polymers is their numerous degrees of conformational freedom, resulting in complex microstructures in the solid state. Understanding charge transport in these systems, which comprises both amorphous and ordered phases with varying degrees of order, is particularly difficult due to the contributions of electronic processes at different length scales². Typically, enhanced mobility results from highly aligned polymer chains, driving interest in the fabrication of highly oriented conjugated polymers. In recent years, extensive research has focused on methods to prepare high-quality conjugated polymer crystalline materials. Techniques such as solution crystallization, spin-coating, and epitaxial crystallization have been developed to regulate their multi-level aggregation processes³. Among them, epitaxial crystallization and topochemical polymerization have become widely used for improving the orientation of conjugated polymers. In this study, we successfully achieved large-area, highly ordered conjugated polymer films on highly oriented substrates using spin-coating and vacuum deposition methods^{4,5}. The photoelectric performance of devices based on these uniaxially ordered films was significantly improved compared to those with the disordered films. This research highlights the importance of preparing high-quality crystalline conjugated polymers for advancing the study of their fundamental physical properties and for the development of high-performance organic optoelectronic devices.

Keywords: Conjugated polymers; Epitaxial crystallization; Topochemical polymerization; Oriented thin film



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DESIGNED AND SYNTHESIS OF ORTHO-SUBSTITUTED CARBAZOLES TWISTER DONOR-ACCEPTOR (D-A) MOLECULES WITH SMALL ΔE_{ST}

Ariffin A^{a,*}, Muhammad-Adzrill MH^a, Woon KL^b, AbdulWahab MK^a,

^aDepartment of Chemistry, Faculty of Science, Universiti Malaya, Kuala Lumpur.

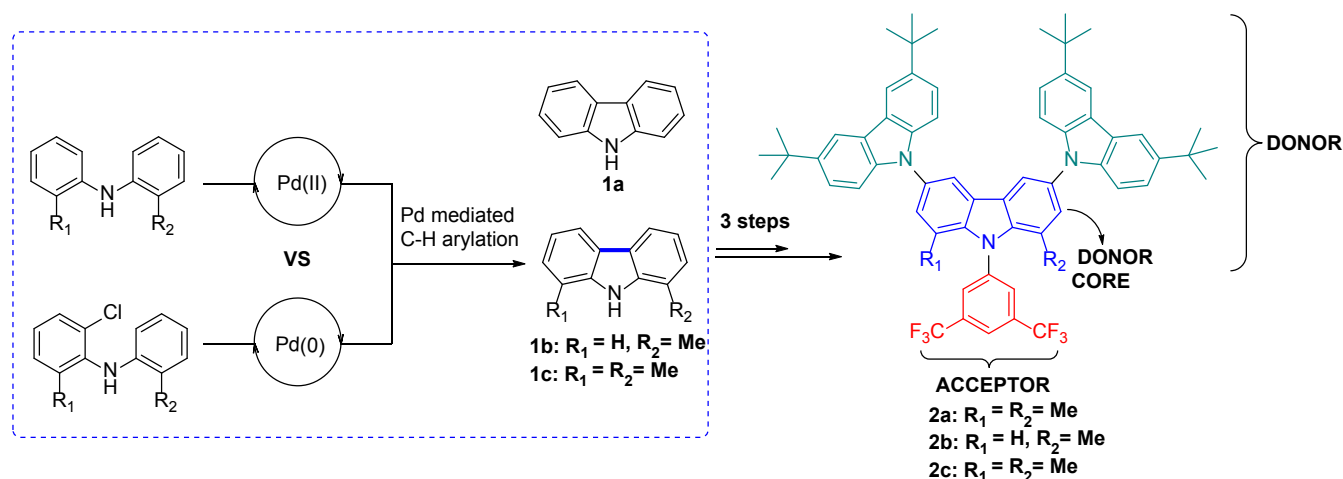
^bDepartment of Physics, Faculty of Science, Universiti Malaya, Kuala Lumpur.

*Corresponding author: azhar70@um.edu.my

Abstract

Carbazoles derivatives are increasingly recognized as an essential building block in the field of optoelectronics due to their low cost and structural versatility, leading to the design of materials with tailored optical and electronic properties [1]. Their high thermal stability, high triplet energies and good charge transport property made them ideal host materials for phosphorescence OLEDs (PHOLEDs) [2, 3]. We designed and synthesized three carbazole-based donor-acceptor (D-A) molecules, labeled **2a**, **2b**, and **2c**, exhibiting progressively lower ΔE_{ST} by modifying the dihedral angle through the introduction of ortho methyl groups in the central carbazole core. The ortho-substituted carbazole cores **1b** and **1c** were synthesized using two distinct palladium-mediated cyclodehydrogenative methods: Pd(II)-catalyzed dual C-H arylation of bisphenylamines and Pd(0)-catalyzed arylation of 2-chlorobisphenylamines. Our results showed that the latter method yields cleaner reactions with higher efficiency. We also present plausible reaction mechanisms for both synthetic approaches, supported by computational studies, to better understand their reactivity and efficiency differences.

Keywords: Carbazole, Donor-Acceptor, OLED, palladium mediated oxidative cyclisation



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DEVELOPMENT OF SUSTAINABLE MATERIALS WITH SELF-HEALING AND CHEMICALLY RECYCLABLE POLYDITHIOURETHANES

Yoshiaki Yoshida^{a,b,c,*}, Tsubasa Sakiyama^a, Ryuichi Suenaga^a

^a Department of Materials Science, Kyushu Institute of Technology

^b Collaborative Research Centre for Green Materials on Environmental Technology

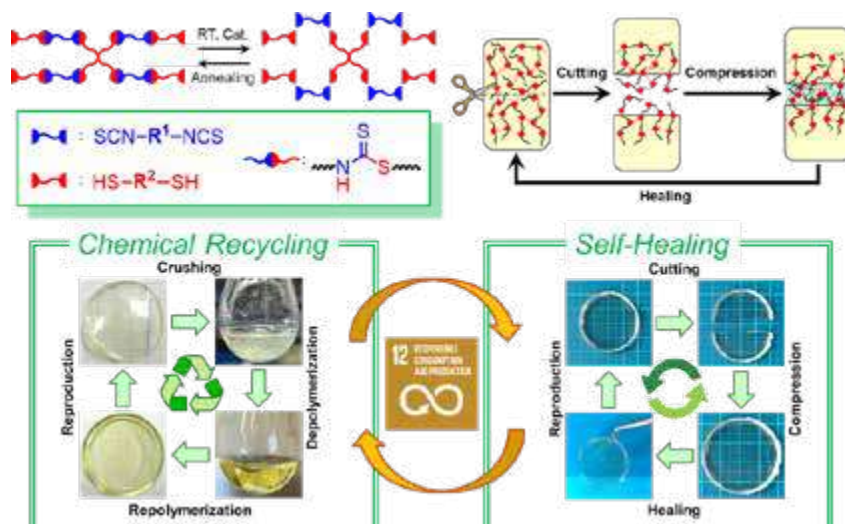
^c PRESTO, JST

*Corresponding author: yoshida.yoshiaki951@mail.kyutech.jp

Abstract

We developed chemically recyclable and self-healable PDTU based on the reversible addition-dissociation reaction and recombinable intermolecular hydrogen bond. Furthermore, the PDTU films apply to optical materials due to their high refractive index and transparency [1, 2]. PDTU is synthesized by the polyaddition of diisothiocyanates and dithiols. The reaction of diisothiocyanates with dithiols proceeds easily at room temperature using a base catalyst to give polymers with high molecular weight. On the other hand, heat treatment of PDTU decomposes it into oligomers with active end groups. Then, the addition of a base catalyst to these oligomers causes the polyaddition to proceed again, yielding a polymer with the same molecular weight as before decomposition. This phenomenon is based on a reversible addition-dissociation reaction between isothiocyanate and thiol groups. We have also shown that the reversible addition-dissociation reaction of isothiocyanates with thiols applies to crosslinked polydithiourethanes synthesized using multifunctional monomers. The PDTU film can be disassembled and regenerated up to at least five times, making PDTU an excellent polymer material for chemical recycling. Furthermore, the PDTU films with an ether structure in the main chain can be joined in a few minutes by pressing the cross sections against each other after cutting, and that the severed sections are completely repaired and recovered to the same strength as before cutting by prolonged standing under ambient temperature and pressure. In this presentation, sustainable features such as self-healing and chemical recycling will be introduced along with the basic properties of PDTU.

Keywords: Sulfur-containing polymers, Self-healing, Chemical recycling, high refractive index



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SELF-ASSEMBLING POLYMERIC BIOMATERIALS FOR CONTROLLED DRUG DELIVERY AND REGENERATIVE MEDICINE

João Borges^{a,*}

^a*CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*

**Corresponding author: joaoborges@ua.pt*

Abstract

Nature provides us with an unprecedented source of fascinating supramolecular systems formed by the supramolecular self-assembly of the fundamental building blocks of life, including saccharides, peptides, nucleobases, phospholipids and their derivatives. Such supramolecular systems include the native extracellular matrix (ECM) of living tissues and organs, formed by the dynamic supramolecular self-assembly and molecular recognition of mainly fibrous proteins, glycosaminoglycans and proteoglycans. This supramolecular biological landscape has inspired scientists to create artificial ECM-mimetic soft self-assembled biofunctional materials to recreate the structural complexity, dynamics, and functional features of the native cellular microenvironment and, ultimately, develop advanced regenerative therapies [1-4].

In this lecture emphasis will be given to the synergistic use of polysaccharides, proteins, peptide amphiphiles, and nucleic acids, as well as molecular self-assembly approaches towards the supramolecular engineering of a library of soft self-assembling polymeric multicomponent biomaterials to interface with living systems. We will discuss how these building blocks can be combined and assembled into bioinspired chemically programmable and dynamic supramolecular polymeric hydrogels/bioinks and biomimetic layer-by-layer-driven soft self-assembling nanobiomaterials to be used as platforms for controlled drug/therapeutics/cell delivery and as bioinstructive matrices to control cell functions in advanced regenerative medicine strategies.

Acknowledgments

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Keywords: Biopolymers, dynamic polymeric hydrogels, layer-by-layer self-assembled nanofilms, drug delivery; cell culture

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VALORIZATION OF WOODY BIOMASS TOWARD A CIRCULAR AND SUSTAINABLE MATERIAL CYCLE

Y. Andou^{a,b,*}, M.A.A. Farid^{a,c}, I. Ibrahim^{a,d}, L. Jacqueline^b

^a Department of Biological Functions and Engineering, Graduate School of Life Science and System Engineering, Kyushu Institute of Technology, 2-4 Hibikino, Wakamatsu-ku, Kitakyushu-shi, Fukuoka-ken, 808-0916, Japan.

^b Collaborative Research Center for Green Materials on Environmental Technology, Kyushu Institute of Technology, 2-4 Hibikino, Wakamatsu, Kitakyushu, Fukuoka, 808-0196, Japan.

^c Institute of Tropical Forestry and Forest Products (INTROP), Universiti Putra Malaysia (UPM), Serdang, 43400, Selangor, Malaysia.

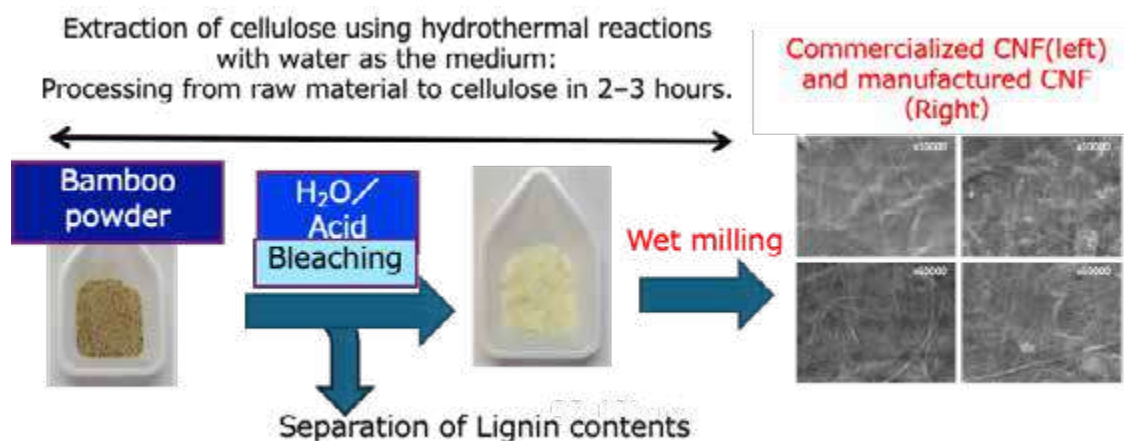
^d Department of Chemical and Environmental Engineering, Faculty of Engineering, Universiti Putra Malaysia, UPM-Serdang, 43400, Selangor, Malaysia

*Corresponding author: ando.yoshito784@mail.kyutech.jp

Abstract

Large quantities of underutilized woody biomass, such as bamboo, oil palm residues, and agricultural waste, remain untapped worldwide despite their potential for high carbon fixation and rapid renewability. Our research aims to establish an environmentally responsible platform for valorizing these abundant resources. Through dilute acid-assisted hydrothermal fractionation, cellulose and lignin are efficiently separated without the use of organic solvents¹. The extracted cellulose is further developed into biodegradable thermoplastic materials and cellulose nanofibers (CNFs)², offering lightweight and high-strength reinforcement for composites. In parallel, lignin is transformed into graphene-based structures through catalytic graphitization³, opening new pathways for sustainable energy and environmental applications. This integrated approach promotes the global transition to a low-carbon circular economy by providing scalable strategies for biomass utilization, ultimately contributing to the realization of carbon neutrality and sustainable societies worldwide.

Keywords: Biomass valorization, Hydrothermal fractionation, Biodegradable thermoplastics, Cellulose nanofibers, Biomass based graphene



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THE NCO CYCLE: A TWO-STEP COMPLETE RECYCLING PROCESS FOR POLYURETHANES

Marthe NEES^{a,*}, Muhammad ADEEL^b, Lukasz PAZDUR^a, Matthew PORTERS^{a,b}, Christophe VANDE VELDE^a & Pieter BILLEN^a

^a *Intelligence in Processes, Advanced Catalysts and Solvents (iPRACS), Faculty of Applied Engineering, University of Antwerp, Groenenborgerlaan 171, 2020, Antwerp, Belgium.*

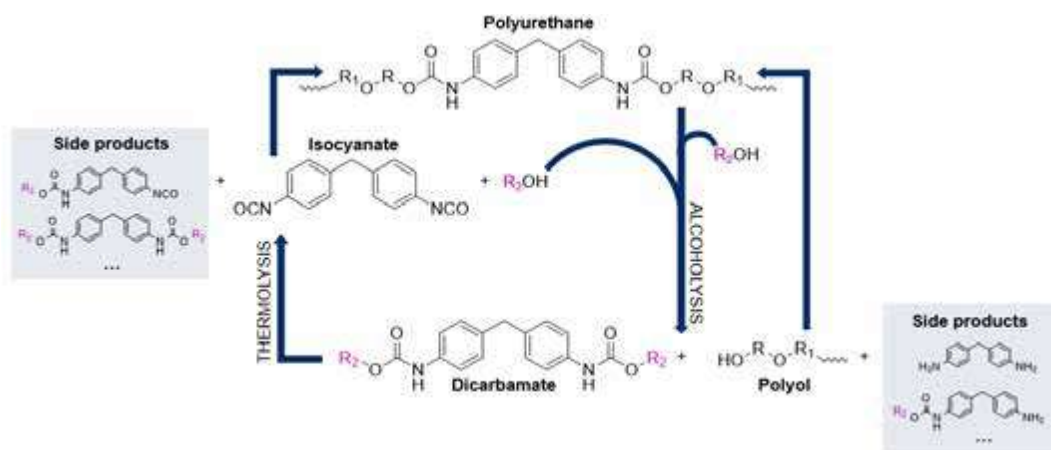
^b *Triple Helix, BlueChem, Olieweg 95, 2020, Antwerpen, Belgium.*

*Corresponding author: marthe.nees@uantwerpen.be

Abstract

Polyurethanes (PU) are a class of mostly thermoset polymers, produced by a reaction of di-(or poly)isocyanates with polyols (polyfunctional alcohols). Since mechanical recycling leads to inferior products, research into chemical recycling methods is on the rise. The most promising chemical recycling technique is split-phase glycolysis, which results in a polyol phase and a glycol/dicarbamate phase [1]. However, to date, this approach only focuses on the recovery of the polyols, neglecting the recycling potential of the dicarbamate phase, which makes up 10-40% of the PU mass. This research has extended the existing alcoholysis processes into a two-step process that can recover both polyols and isocyanates. This was achieved by a thermolysis reaction after the alcoholysis reaction, applied to the previously ignored carbamate phase to regenerate isocyanates without the use of toxic phosgene gas [2]. Since the carbamate bond is thermally reversible [3], the thermolysis step can take place at relatively low temperatures (ca. 200°C). This is a pioneering step towards the complete recycling of polyurethanes, as well as the production of PU from recycled materials. As such, both the polyols and isocyanates can be used in the synthesis of new PU. The first experiments of the recycling process using isopropanol were successful in recovering the polyols and a small amount of isocyanates. The thermolysis of the generated isopropyl-carbamate at 275°C for 10 minutes successfully recovered isocyanates with a yield of 35%. The study also revealed the presence of various by-products, including polycarbodiimide, which was confirmed by FTIR and contributes to the complexity of the thermolysis mixture. Thus, the proposed recycling process offers a sustainable solution for PU foam waste by effectively utilizing the carbamate fraction without relying on energy-intensive methods or toxic reagents, thus using green chemistry to contribute to a more sustainable future.

Keywords: Alcohols • Isocyanates • Polymers • Sustainable Chemistry • Thermolysis



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EFFECT OF CHEMICAL MODIFICATION ON DATE PALM FIBERS

Helanka J. Perera^{a,*}, Anjali Goyal^b, Saeed M. Alhassan^b

^a Chemical Engineering Department, Abu Dhabi Campus, Higher College of Technology, Abu Dhabi, United Arab Emirates

^b Department of Chemical Engineering, Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates

^c Affiliation author W.

*Corresponding author: hperera@hct.ac.ae

Abstract

Recently, great interest was paid to natural fibers while developing new technologies by considering the environmental aspect. These new technologies will enable us to properly utilize available natural resources and waste management. The application of natural fibers in industries has taken great attention in the last few years as an alternative to glass or carbon fibers. Date palm fibers (DPF) are a good substitute for synthetic reinforced fibers. The properties of the DPF composite depend on the interfacial bonding between fibers and polymer matrix. This interfacial bonding can be increased by treating the natural fibers with fluoro and non-fluoro silane coupling agents. Modifying the final properties of treated fibers are very important when used in various applications. Thermal property is one of the leading property gives an idea of the stability of the material with temperature fluctuation. Raw DPF underwent different surface modifications during this study with different silane help. Modified DPFs will be characterized using thermal gravimetric analysis to know the thermal stability. Scanning electron microscope and X-diffraction help to understand the morphology and crystallinity.

Keywords: Date palm fiber, silane coupling agents, thermal gravimetric analysis, cellulose, hydrophobicity

Graphic / Image

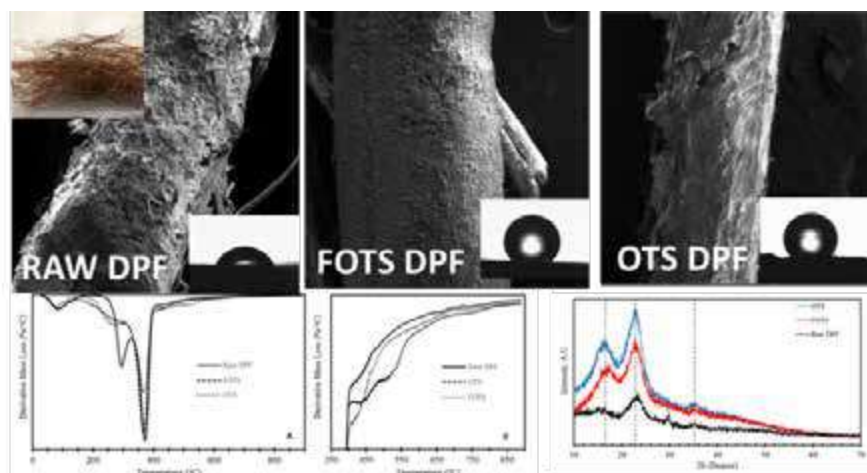


Figure. Scanning electron microscope images and thermal gravimetric analysis of raw DPF, fluoro DPF (FOTS) and non-fluoro DPF (OTS).

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SYNTHESIZING POLYFULLERENES SUSTAINABLY

Vitor Fernandes Moreno^{1,2}, Eleftheria Batagianni¹, Douvotsu Elisa MOUNGADJI Bouassa¹, João Victor Morais Lima², Silvia Letícia Fernandes^{2,3}, Um Kanta Aryal⁴, Luiz Carlos da Silva Filho², Deuber Lincon da Silva Agostini⁵, Didier Bégue¹, Clarissa de Almeida Olivati⁵, Patricia Targon Campana⁶, Morten Madsen⁴,
Carlos Frederico de Oliveira Graeff², Roger C Hiorns¹

¹CNRS/Univ Pau & Pays Adour, Institut des Science Analytiques et Physico-Chimie pour l'Environnement et les Matériau, France. ²FCT/Unesp - Faculdade de Ciências e Tecnologia (Bauru Campus), Brazil ³ONINN – Centro de Inovações, Brazil. ⁴Mads Clausen Institute, SDU Denmark.

⁵UNESP - Faculdade de Ciências e Tecnologia (Presidente Prudente Campus), Brazil.

⁶University of São Paulo (School of Arts, Sciences, and Humanities), Brazil.

*Corresponding author: roger-clive.hiorns@cnrs.fr

Abstract

Main-chain fullerene-based polymers[1] are still rare, however, they are gaining interest for their use in photovoltaics and organic electronics. For examples, recent work has demonstrated their use as interlayers in perovskite solar cells to give efficiencies around 23% [2] and exceptional stabilities in organic solar cells [3]. They might also find use in ammonia sensors [4] and in drug delivery systems. The key properties that these materials exhibit is their combination of fullerene's extraordinary ability to accept electrons, and their polymeric capability to make thin films from solution that are smooth compared to films from fullerenes alone. This said, the methodology used to make these polymers can impact extremely heavily on its final physico-chemical properties. Therefore in this presentation we review the various types of poly(fullerene)s and their structures, and disclose new ways of making them, focussing on methods that are sustainable. We also look at ways of making amphiphilic poly(fullerene)s which are not only sustainable but also have properties tailored for solar cell and drug delivery technologies. Finally we also show some examples of their use in organic and perovskite solar cells.

Keywords: poly(fullerene); polymer chemistry; organic photovoltaics; perovskite solar cell; macromolecules

Graphic / Image



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3D-PRINTABLE POLYMER NANOCOMPOSITES, WITH HIGH THERMAL CONDUCTIVITY AND VERY LOW ELECTRICAL CONDUCTIVITY

SIMONATO Jean-Pierre^{a,*}, PIETRI Thomas^a, BODIN Antoine^a, CELLE Caroline^a

^aUniv. Grenoble Alpes, CEA, LITEN, F-38000 Grenoble, France.

*Corresponding author: jean-pierre.simonato@cea.fr

Abstract

Due to the advancements in fast charging technologies such as high energy density batteries the high heat generation while in operation becomes very intense. Besides high thermal conductivity needed to dissipate heat, good electrical insulation is also required to avoid electrical issues.

The use of thermoplastic polymers appears relevant due their intrinsic electrical insulation behavior and easy processability. However, such materials generally present intrinsic low thermal conductivity.

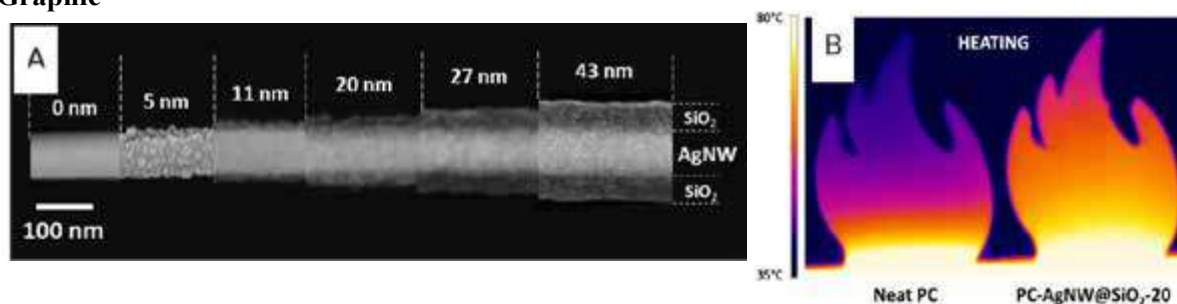
We developed a new strategy to incorporate thermally conductive yet electrically insulating fillers to a polycarbonate matrix, with care to ensure 3D printability.

In this presentation, we will show that the development of one-dimensional silver nanowires coated with a thin layer of silica (AgNW@SiO₂) allows the fabrication of very efficient heat dissipative 3D printable nanocomposites.

We will show how the fine tuning of the silica shell on silver nanowires plays a critical role to reach excellent performances, and how the 3D printing is important. Indeed, the resulting orientation and alignment of the nanofillers provided by the 3D printing technique led to remarkable in-plane thermal conductivities, up to 3.48 ± 0.06 W m⁻¹ K⁻¹, while keeping an electrically insulating property. This led to a 15-fold improvement of the thermal conductivity compared to the pristine polymer matrix.

Keywords: Nanocomposites, 3D printing, Heat dissipation, Electrical insulation, Core-shell nanoparticles

Graphic



A) Core-shell Ag@SiO₂ nanowires; B) Thermal images of 3D-printed flames of the polymer matrix(PC) and the nanocomposite, showing different thermal conduction

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MOLECULARLY IMPRINTED POLYMERS IN ADVANCED ENVIRONMENTAL SENSING USING FAPA-MS

Aleksandra Lusina^{a,*}, Michał Cegłowski^a

^aAdam Mickiewicz University, Uniwersytetu Poznańskiego 8, Poznań, Poland

*Corresponding author: aleksandra.lusina@amu.edu.pl

Abstract

Molecularly Imprinted Polymers (MIPs) are specialized materials designed to recognize and selectively bind specific molecules through template-shaped cavities formed during polymer synthesis ¹. These cavities precisely match the size, shape, and functional groups of the target molecules, enabling unique selectivity ². Thanks to their high recovery rates, repeatability, and cost-effectiveness, MIPs are increasingly being integrated into smart device designs as molecular recognition elements for real-time analysis ³⁻⁴.

A revolutionary application of MIPs is their integration with Flowing Atmospheric-Pressure Afterglow Mass Spectrometry (FAPA-MS), a rapid, preparation-free analytical technique. It excels in the direct detection of trace analytes in complex environmental matrices, offering mass spectrometry spectra acquisition in seconds. This approach improves pollutant detection in diluted solutions and solid-phase samples, changing environmental testing with its high sensitivity and efficiency ⁵.

The focus of the research is the development of MIP-based sensors for detecting substances of environmental concern, including herbicides (MCPA), fluorinated surfactants (PFOS), explosives (RDX), and preservatives (propylparaben). By combining the specificity of MIPs with the innovative capabilities of FAPA-MS, this method achieves remarkably low detection limits (LODs), making it easier for next-generation environmental monitoring systems. This work highlights the transformative potential of MIP-based sensors, showcasing their versatility and precision in addressing pressing environmental challenges. This work shows how new methods are changing the way we detect harmful substances in real-world environmental situations.

Keywords: Molecularly Imprinted Polymers, FAPA-MS Technique, Rapid and Selective Determination, Environmental Water Treatment, Limit of Detection (LOD)

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SOL/GEL TRANSITION OF THERMORESPONSIVE ALGINATES: FROM LIQUIDS TO ELASTIC AND STICKY MATERIALS

D. Hourdet*, L. Barbier, P. Pipart, H. Guo, M. Vahdati, G. Ducouret, Y. Tran

SIMM, ESPCI Paris, PSL University, Sorbonne University, CNRS, F-75005 Paris, France

*Corresponding author: dominique.hourdet@espci.fr

Abstract

Associating polymers have known a large development due to their high performances as thickeners in aqueous media with important applications in various domains like oil recovery, cosmetics or paints. With time the systems become more efficient, even smart as they are able to change their properties under controlled environment. This is the case of responsive polymers which respond to stimuli like salt, pH, temperature, light or external fields. Under controlled conditions, these systems readily form physical networks or nanostructures which offer wide potentialities in biomedical engineering. In this context, biopolymers have an important role to play and we are currently developing a platform of responsive polymers by grafting thermoresponsive LCST side-chains onto polysaccharides.¹⁻³ In this work, thermo-associating copolymers were prepared by grafting poly(N-isopropylacrylamide) (PNIPAM) onto a rich-mannuronic alginate backbone (ALG).^{1,3} Viscoelastic analyses demonstrate that ALG-g-PNIPAM self-associate reversibly and form gels in semi-dilute solutions either by cooling or heating depending on the ionic environment (**Figure 1**). As the aggregation process of ALG and PNIPAM depends mainly and respectively on the nature of cations and anions, the choice of the salt is critical to control the self-assembling behavior. Complementary experiments, performed by DSC and NMR, confirm the close relationship between the self-association of LCST grafts, forming micro-domains, and the macroscopic properties. Viscoelastic studies, initially performed in the linear regime, were extended to large deformations using steady state analysis and tack experiments to investigate adhesive properties. The thermo-associative behavior of these copolymers, whose properties can be finely tuned in order to form sticky gels at body temperature, clearly demonstrates their potential in biomedical applications such as injectable gels for drug delivery or tissue engineering.³

Keywords: alginate, thermo-responsive polymers, gelation, injectable hydrogel

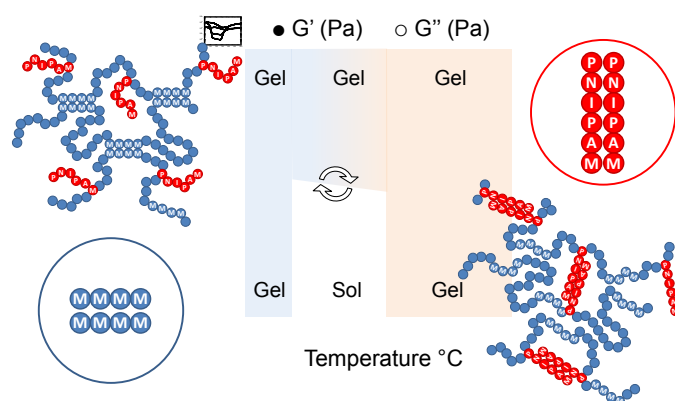


Figure 1: Gel/Sol/Gel transitions of aqueous solutions of ALG-g-PNIPAM in the presence of salts.¹

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SYNTHESIS AND CHARACTERIZATION OF NOVEL COPOLYMERS OF POLYACETYLENE AND PDI-CONTAINING POLYOLEFINS USING ROMP

Hassan S. Bazzi^{a,*}, Santhosh K. Podiyanachari^b, Maciej Barlog^b, Mohammed Al-Hashimi^a

^aCollege of Science and Engineering, Hamad Bin Khalifa University, Doha, Qatar

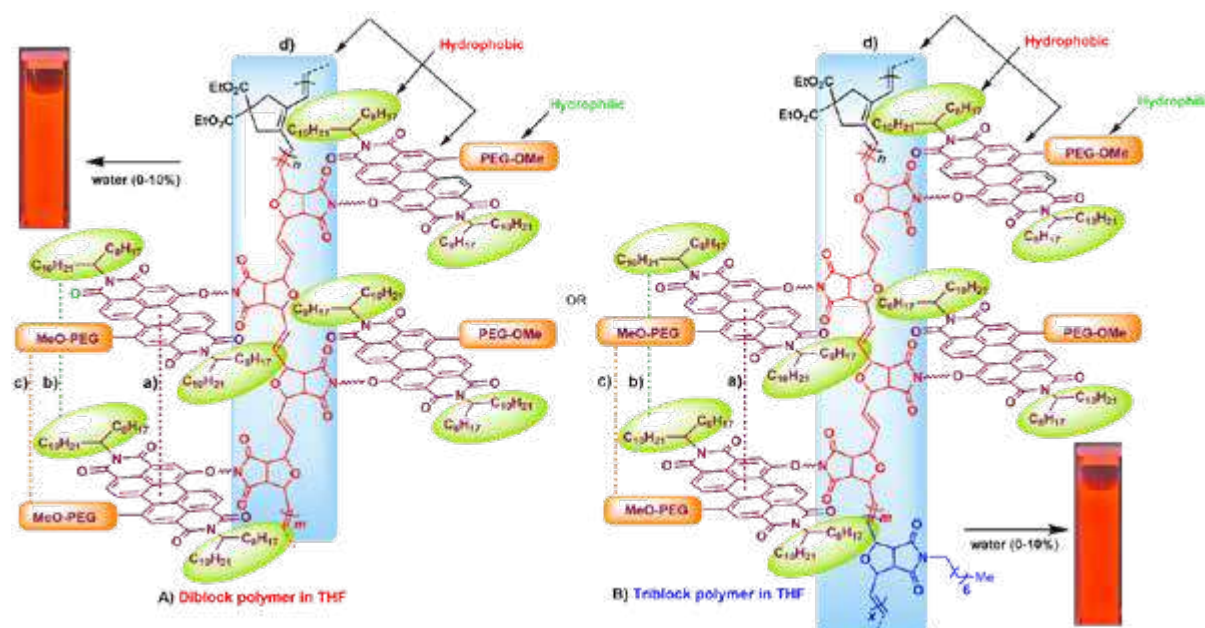
^bTexas A&M University at Qatar, Doha, Qatar

*hbazzi@hbku.edu.qa

Abstract

Amphiphilic copolymers of highly conjugated poly(acetylene)s and poly(ethylene glycol)-functionalized perylene diimide poly(olefin)s have been synthesized via tandem cyclopolymerization and ring-opening metathesis copolymerization (ROMCP) methodologies. The relative atomic weight percentages of both di- and tri-block copolymers were estimated using XPS analysis. Photophysical properties of both copolymers have been explained based on both UV-Vis and fluorescence spectroscopic analysis shedding more light on their different stages of organization as well as the π - π stacking interactions of the PEG750-incorporating perylene cores in aqueous solutions. Copolymeric surface analysis, segmental patterns and film morphology were examined by AFM revealing globular or spherical morphological features enhanced by various functional groups present in the polymer bulk. In addition, the formation of these spherical morphologies was further visualized in the thin film cross-sections of both di- and tri-block polymers by SEM to confirm the surface morphologies determined by AFM analysis of both polymeric materials.

Keywords: olefin metathesis, ROMP, cyclopolymerization, perylene diimide, conjugated polymers



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ENHANCED PHOTOREFRACTIVE PERFORMANCE VIA TAILORED CONJUGATION LENGTH AND DENSITY OF STATE IN POLY (CARBAZOLYL-AMINE) POLYMERS

Meng-Che Tsai^{a*}, Kuan-Hsun Wu^a, Satoshi Wada^b, Masaki Horie^a, Takafumi Sassa^b

^aDepartment of Chemical Engineering, National Tsing Hua University, Taiwan (R.O.C.)

^bPhotonics Control Technology Team, RIKEN Center for Advanced Photonics, RIKEN, Japan

*Meng-Che Tsai: allentsai0208ms@gapp.nthu.edu.tw

Abstract

In our previous research, organic photorefractive materials based on poly(carbazolyl-amine) host polymers demonstrate excellent solid-state compatibility with functional additives and high hole mobility. Furthermore, the crystallinity of the PR composite and the ion migration speed in PR devices can be modulated through incorporating biphenyl groups in random co-polymers.^[1] The enhanced PR performance is achieved with ion-assisted space-charge-limited current in amorphous phase and wider width of density of state (DOS). Consequently, the milestone performance for organic PR materials is realized with a response time of 3.8 ms and a sensitivity of $16.7 \text{ cm}^3 \text{ kJ}^{-1}$, which are comparable to the benchmarks of inorganic PR crystals $\text{Sn}_2\text{P}_2\text{S}_6$ and $\text{Bi}_{12}\text{SiO}_{20}$. In this study, fundamental research in tailoring the DOS width and conjugation length is conducted through increasing the molar ratio of biphenyl groups and replacing the backbone of polymers with 2,2'-dimethylbiphenyl and 3,9-indolocarbazole groups, respectively. The results are expected to provide insight strategies for designing efficient charge-trapping PR polymers with sub-millisecond response time and high PR sensitivity.

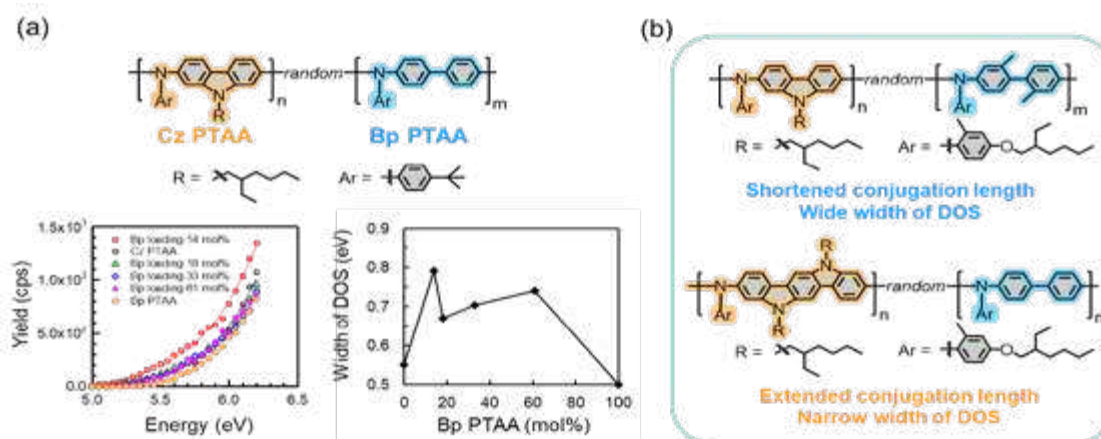


Figure 1. (a) Dependence of DOS width on Bp PTAA ratios. (b) Effect of molecular design on conjugation length through and DOS width.

Keywords: Organic photorefractive device, density of state, conjugated polymers.

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PRINTABLE 2D NANOPARTICLE SUPERLATTICES VIA DIRECTED CONFINED SELF-SEMBLY OF POLYMER-TETHERED NANOPARTICLES

Renhua Deng^{a*}

^a School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, No. 1037
Luoyu Road, Wuhan, 430074, China.

*Corresponding author: rh Deng@hust.edu.cn

Abstract

Polymer-tethered nanoparticle (NP), acting as a special building block, could mimic block copolymer to self-assemble into ordered hierarchical structures. Due to their combined unique properties of NPs and excellent mechanical property of polymers, their 2D assemblies have attracted intensive attentions.

We introduce a series of 2D monolayer NP superlattices with polymer-tethered Au NPs by utilizing direct-ink-writing technology, which can supply an impervious space and drive directed self-assembly of NPs. We study the contact angle and concentration of ink, dry rate and move speed of three phase contact line on morphology of NP deposits. The interparticle distance and number density of NPs can be effectively tuned by tailoring the polymer chain length and grafting density. This printing strategy is general and can be applied to NPs with different shapes and sizes. These 2D NP superlattices can server as nanofloating gate array and dielectric medium for memory devices and other applications.

Keywords: Nanoparticles, Polymer-grafting, Self-assembly, 2D superlattices, Memory devices

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SOLVENT ACIDOLYSIS CRYSTALLIZATION OF HALIDE PEROVSKITE SINGLE CRYSTALS

Ahmed L. Abdelhady

Department of Chemistry, Khalifa University, Abu Dhabi, 127788 UAE

Corresponding author: ahmed.abdelhady@ku.ac.ae

Abstract

We introduce a novel solvent acidolysis crystallization (SAC) technique for the synthesis of methylammonium (MA) lead halide perovskites, where the hydrolysis of N-methylformamide (NMF) in acidic conditions forms the MA cation in situ.[1] Bulk crystals were grown at room temperature without the need for antisolvents, simplifying the process and reducing the use of toxic and expensive chemicals. The SAC technique also facilitated the creation of MAPbBr₃ single crystals with intense edge emission under UV light.[2] Micro-X-ray diffraction revealed that lattice compression at the edges correlated with longer-lived photogenerated carriers and enhanced detectivities in planar photodetectors. Furthermore, we synthesized mixed dimethylammonium/methylammonium lead tribromide (DMA/ MAPbBr₃) crystals, achieving 44% DMA incorporation while maintaining the 3D cubic phase.[3] These mixed crystals exhibited suppressed orthorhombic phase and lower phase-transition temperatures, with higher detectivity at room temperature and significant enhancement below 200 K.

Our research also addressed the formation of metallic lead in perovskite crystals, finding that precursor solution composition and concentration played a crucial role.[4] Black-colored mixed DMA/ MAPbBr₃ crystals, despite their unexpected coloring, showed higher crystallinity and fewer defects, underscoring the need for further investigation into precursor solution chemistry.

Additionally, we developed a surface engineering crystallization technique to grow a polycrystalline MAPbBr₃ film on bulk single crystals, resulting in intense green emission under UV light.[5] These surface-engineered crystals exhibited fewer surface defects and significantly improved X-ray detector sensitivity. The polycrystalline nature and surface engineering of MAPbBr₃ single crystals proved essential for superior optoelectronics, achieving high detectivities and photoresponsivities.[6] This highlights the potential of the SAC technique for advancing the synthesis and application of halide perovskites in optoelectronic devices.

Keywords: Halide Perovskite; Single Crystals; Crystallization; Optoelectronics

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SOLAR INTERFACIAL EVAPORATORS BASED ON BIOMATERIALS

Weiwei Shi^{a*}, Xiaxia Yang^a, Tianxin Lu^a, Yu Zhou^a,

^a*Division of Natural and Applied Sciences, Duke Kunshan University*

^{*}*Corresponding author: ws183@duke.edu*

Abstract

Interfacial solar evaporation is an innovative technique that has garnered significant attention for its potential applications across a variety of fields. The technology's attractiveness lies in its use of renewable energy and its potential to address critical issues such as water scarcity and sustainable energy generation. By integrating advanced materials and innovative system designs, interfacial solar evaporation can be tailored to meet the specific demands of these diverse applications, e.g., wastewater treatment, water desalination, and energy production. Solar interfacial evaporators that incorporate biomaterials are at the frontier of sustainable technology, leveraging natural materials and designs to improve the efficiency and environmental friendliness of water evaporation processes. The preliminary results showed that the evaporation rates of bio-inspired interfacial evaporators have achieved multiple times better, compared to the control groups of pure water or saline water. Both the solar evaporation and water desalination performance have been enhanced significantly at the one solar irradiation. The use of biomaterials in solar interfacial evaporators presents multiple advantages, including sustainability, biodegradability, and often a lower carbon footprint in their manufacturing. As research in this area progresses, it's expected that the use of biomaterials will enable the design of even more innovative and eco-friendly solar evaporation systems.

Keywords: Solar Evaporation, Water Desalination, Bio-Inspiration, Sustainable Energy

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MACHINE LEARNING-BASED PREDICTION OF Mg-CONTAINING MATERIALS

Mengfan Tang¹, Yu Tian¹, Guang Zheng^{*1}

*Key Laboratory of Optoelectronic Chemical Materials and Devices of Ministry of Education, Jiangnan University,
Wuhan, Hubei 430056, China*

**Corresponding author: mzheng88@foxmail.com*

Abstract:

Based on goal-oriented machine learning (ML) simulations and the density functional theory (DFT) method, we have calculated several important parameters for some Mg-containing candidate materials as high performance cathode materials, including band gap, diffusion activation energy, diffusion coefficient, ionic conductivity, and thermal stability at room temperature. The results exhibited that the Mg-containing materials have excellent performance in terms of electronic conductivity, ionic conductivity, coefficient of thermal expansion, and stability.

Keywords: machine learning(ML), density functional theory(DFT), cathode materials

CHITOSAN FROM EXTRACTED CHITIN OF *SARDINELLA LEMURU* (TAMBAN) FISH SCALES

Almer Chris C. Tuayon^a, Sheeva M. Yahcob-Saddalani^{a,*}

^aChemistry Department, College of Science and Mathematics, Western Mindanao State University.

*Corresponding author: sheeva.saddalani@wmsu.edu.ph

Abstract

Chitosan, a versatile biopolymer, is derived from chitin, a natural polysaccharide found in various sources, including fish scales. This study focused on producing chitosan from *Sardinella lemuru* scales and characterizing it using Fourier Transform Infrared (FTIR) analysis, comparing its properties to commercial chitosan. The objectives were to extract chitin from fish scales using optimal deproteinization and demineralization parameters, determine the effective ratio of chitin to sodium hydroxide (NaOH) for chitosan production based on yield and degree of deacetylation (%DD), and characterize the extracted chitosan via FTIR Spectroscopy.

The produced chitin had a protein content of 15.5% and calcium content of 3.86%. Chitin was then deacetylated using ratios of 1:5, 1:10, and 1:20 of chitin to 45% NaOH solution. FTIR analysis revealed minimal spectral shifts and relatively higher peaks at N-H stretch and O-H stretch (3200-3550 cm⁻¹), C-N stretch of amide II (1470-1570 cm⁻¹), and C-O stretch (1050-1085 cm⁻¹) for each ratio variation. Significant differences between chitin and chitosan were observed at 3350-3500 cm⁻¹, indicating greater deacetylation in chitosan due to O-H stretching overlap with N-H stretching. The 1:10 ratio yielded the highest chitosan yield of 87.35% and a degree of deacetylation of 72.80%. These findings suggest that *Sardinella lemuru* scales are a viable source of chitosan. With a higher %DD, the produced chitosan could possess high solubility and strong cationic character, making it suitable for applications in drug delivery, gene delivery, and tissue engineering.

Keywords: Chitin, Chitosan, Fish Scales, Degree of Deacetylation, FTIR Spectroscopy

FUNCTIONALIZED BIO-COPOLYMERS FOR NUTRIENT PRESERVATION OF HIGH PROTEIN FOOD

Jiahui Du ^a, Xueyan Yun ^a, Tungalag Dong ^{a*}

^a College of Food Science and Engineering, Inner Mongolia Agricultural University

*Corresponding author: dongtlg@163.com

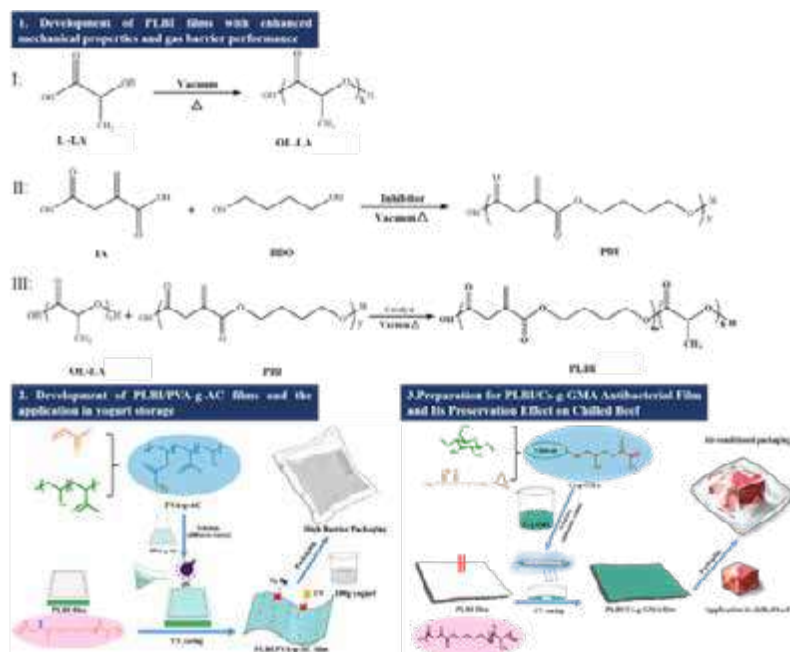
Abstract

Poly (l-lactic acid) (PLLA) as one of the most promising alternatives to petroleum-based materials has attracted significant attention from researchers. Our research focuses on developing modified PLLA-based packaging materials. Given PLLA's low toughness and moderate barrier properties, we introduced active groups such as poly (butylene itaconate) copolymer (PBI) into the PLLA backbone. This led to the synthesis of poly (lactic acid-butylene itaconate) (PLBI) copolymers, which exhibit excellent toughness and gas barrier properties. Based on this, the grafting of functional substances can be further implemented to achieve additional modifications. The performance of these new materials has been comprehensively evaluated and applied in food preservation and storage. In this context, several key points merit further discussion.

1. Development of PLBI films with enhanced mechanical properties and gas barrier performance ¹.
2. Development of PLBI/PVA-g-AC films and the application in yogurt storage ².
3. Preparation for PLBI/Cs-g-GMA antibacterial film and its preservation effect on chilled beef ³.

As a result, PLLA-based packaging films with enhanced barrier performance and antibacterial properties have been successfully developed.

Keywords: polylactic acid-based composite film, high barrier packaging, antibacterial packaging, grafting



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PERFORMANCE EVALUATIONS OF POLYURETHANE FILMS SYNTHESIZED FROM CASTOR OIL AS PART OF THE POLYOLS IN LINE WITH POLY(TETRAHYDROFURAN) POLYOL

Kai Yi Wong^a, Min Rui Chia^b, Seng Neon Gan^c, Sook-Wai Phang^{a*}, Sau Leng Sin^{a*}

^a Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Kelang, Setapak, 53300 Kuala Lumpur, Malaysia

^b Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600, Bangi, Selangor Darul Ehsan, Malaysia

^c Department of Chemistry, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia

Corresponding authors: pinktphang@gmail.com, sinsl@tarc.edu.my

Abstract

The use of bio-based polyols from vegetable oils have gradually become an interesting approach to produce polymer. Castor oil is one of the examples that have been widely used as biobased polyols in the synthesis of polyurethanes as part of the renewable resources. A series of castor oil-based polyurethanes (PUs) with replacing part of the conventional polyol [poly(tetrahydrofuran)] by castor oil were synthesized and study its performance as PU films. The elongation at break and tensile strength did not follow a straight increase with percentage of castor oil. Incorporation 20% of castor oil has shown the maximum elongation at break with 496.88% whereas replacement of 50% castor oil exhibited highest tensile strength of 20.28 MPa which is slightly higher than incorporation of 20% castor oil (19.84 MPa). The glass transition temperature (T_g) has shown significant increase from -39 °C with replacement of 10% castor oil to -9 °C with replacement of 50% castor oil. The first degradation temperature of the castor oil-based PUs was found to decrease between 2.57% to 4.82% compared to pristine PU with the increase of castor oil to 50%. The increase in the amount of castor oil resulted in an improvement in the water-resistant behaviour of the resulted PU films. The percentage of water absorption was gradually decreased from 1.47% for pristine PU to merely 0.75% as the amount of castor oil increased from 0% to 50%.

Keywords: polyurethanes, castor oil, mechanical properties, water-resistant

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DEVELOPMENT OF SUSTAINABLE MATERIALS BY INCORPORATING WASTE ALKALINE SLUDGE FOR CO₂ CAPTURE

Siti Sarahah Sulhadi^{a,*}, Azizul Hakim Lahuri^a and Syawal Mohd Yusof^a

^a Department of Science and Technology, Faculty of Humanities, Management and Science, Universiti Putra Malaysia Bintulu Campus, P.O Box 396, Nyabau Road, 97008 Bintulu, Sarawak, Malaysia

*Corresponding author: azizulhakim@upm.edu.my

Abstract

Global CO₂ emission had reached a new record high of 37.4 billion tonnes at 2024 1 and it is projected to only increase from this point. Carbon Capture and Storage (CCS) was proposed to tackle this particular problem to prevent the global temperature from exceeding 1.5 °C from the current temperature. CO₂ capture under CCS plan garners much attention as it involves reducing greenhouse gas that currently is the culprit of continuous global warming. Some studies also have found a strong correlation between higher CO₂ concentrations and stronger weather events such as hotter summers, heat stress, and extreme tropical precipitation 2. This study explores the possibility of the development of cellulose with alkaline sludge (AS) as an efficient material for CO₂ capture. Cellulose was chosen as it is sustainable, renewable, and relatively economical 3. The hydroxyl group in cellulose furthermore can help with CO₂ adsorption 4 5. Cellulose and AS share the economical feature if upscaling were to happen. AS utilization can be understood as sustainable and reducing the wastage from industry. Samples were prepared following simple dissolvment of cellulose and then adding the calcined AS. Different concentration of cellulose was prepared with AS to help with CO₂ adsorption efficiency. Prepared samples then undergo characterization analysis including X-Ray Fluorescence (XRF), X-Ray Diffraction (XRD), N₂ adsorption-desorption analysis, CO₂ adsorption-desorption analysis, Fourier Transform Infrared (FTIR) and Field Emission Scanning Electron Microscopy (FESEM). The highest CO₂ adsorption capacity was shown by sample 2.5C_1AS with 6.14 mg/g with the surface area of only 0.35 m²/g at 25 °C. This study found that the addition of AS and a high concentration of cellulose had generated large pores that helped improve the sample with CO₂ uptake 6.

Keywords: cellulose, alkaline sludge (AS), CO₂ adsorption

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THERMAL DIFFUSION PROCESSES IN POLYMER COMPOSITES BASED ON *N,N*-DIETHYL-3-METHYLBENZAMIDE

Sergei Zverev^{a,*}

^a *Disinfectology Institute of F.F. Erisman FSCH of Federal Service for the Oversight of Consumer Protection and Welfare of the Russian Federation*

*Corresponding author: zverev.s.chem01@gmail.com

Abstract

Polymer composites containing repellents against blood-sucking insects are used to make protective materials. This study details the preparation of *N,N*-diethyl-3-methylbenzamide-based (DEET) composites using various approaches and the study of thermal diffusion processes of the repellent. The first approach is the development of material on the inorganic sorbents, which are incorporated in a polymer layer. Previously, data was obtained on the sorption activity of zirconia, alumina and silicas on repellents¹. The polymer used was a copolymer of polyacrylic acid, which is widely applied in protective textile materials. The thermal diffusion rate of the repellent was studied by heating the polymer composite². Another approach is to obtain electrically conductive polymer composites based on DEET repellent³. A polymer composite that conducts electricity at low voltages can be obtained by incorporating multi-walled carbon nanotubes. This allows heating of the composite to release the repellent from the surface of the material. In addition, this material has a high degree of flexibility. The thermal diffusion properties of the repellent in different shapes have also been described.

A detailed study of the thermal diffusion of repellents will allow the development of materials that are effective against insect attack.

Keywords: thermal diffusion, polymer composites, repellents, sorbents, electrical conductivity

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IONIC LIQUID CRYSTALS AS ELECTROLYTES: FROM SOLID TO LIQUID FORMULATIONS

Andreia F. M. Santos ^{a,*}, Daniela M. Correia ^b, Senentxu Lanceros-Mendez ^{b,c}, Maria H. Godinho ^d,
Madalena Dionísio ^a, Luis C. Branco ^a

^a LAQV-REQUIMTE, Department of Chemistry, and ^d i3N/CENIMAT, Department of Materials Science, NOVA School of Science and Technology, NOVA University of Lisbon, 2829-516 Caparica, Portugal.

^b Centre of Chemistry, University of Minho, 4710-057 Braga, Portugal.

^c BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain.

*Email: afm.santos@fct.unl.pt

Abstract

Ionic liquid crystals (ILCs), a class of advanced materials whose properties can be tuned by the wise pairing of the cation and anion, have emerged as promising candidates for different applications, combining the characteristics of ionic liquids and liquid crystals. Recently, a family of pyridinium and picolinium ILCs was synthesised and characterised in terms of their mesomorphic behaviour and conductivity profile [1–3]. These materials were explored in different ways, including their confinement in an inorganic silica matrix to obtain hybrid solid-like materials capable of being used as solid electrolytes. In this context, three composites were prepared at different guest-host fractions and investigated by a sum of techniques [4]. It was possible to achieve green and economically viable composites with greater thermal resistance, better conductivity and lower resistance at 20 °C, using a lower amount of ILC [4]. On the other hand, the potential of such pyridinium and picolinium ionic liquid crystals as liquid electrolytes for electrochromic devices was investigated. To do that, task-specific electrolytes were developed to dissolve responsive probes and their performance was evaluated in display devices. This work demonstrates the versatility of ionic liquid crystals, disclosing also some sustainable strategies to improve their performance, which can be extrapolated to other materials.

Keywords: ionic liquids, ionic liquid crystals, solid electrolytes, liquid electrolytes, sustainable materials

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FAST LOSSY SRIDHARA-BASED COMPRESSION AND EIGENSOLVING OF CIRCUMCORONENE HAMILTONIANS FOR QUANTUM SENSING

Dennis Lima^{a,*}, Saif Al-Kuwari^a

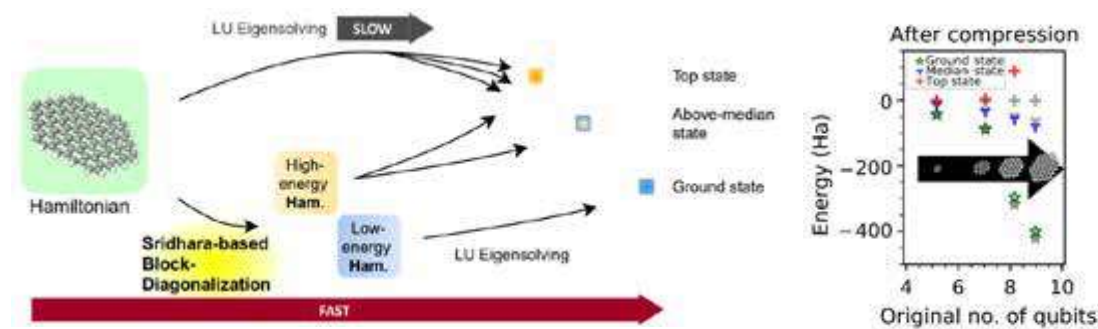
^a Qatar Center for Quantum Computing, College of Science and Engineering, Hamad Bin Khalifa University.

*Corresponding author: deaq54989@hbku.edu.qa

Abstract

Graphene-based photocathodes are part of a new line of sensors under simulation and assessment for implementation in detectors at CERN due to their lightweight and high efficiency¹. To push the simulation of such complex sensors in quantum computers closer to reality, fast matrix compression techniques that preserve eigenvalues are needed, but the best candidates^{2,3} rely on subroutines of either QR or LU algorithms. We extend Sridhara's equation⁴ for the root of a quadratic polynomial by flexibilizing the block-determinant formula to allow for the block-diagonalization of the Hamiltonians of benzene, coronene, circumcoronene and circumcircumcoronene in STO-3G basis and B3LYP functional. We achieved performance 9.9897 times faster than the LU eigensolver alone due to the compression of circumcircumcoronene's Hamiltonian from nearly $2^{8.977}$ to 2^2 in matrix dimensions (99.21% reduction). The exponential speedup as a function of the matrix size, and small error of 4.86%, suggest that the Sridhara-based block-diagonalization routine can efficiently reduce the search space in quantum simulation of graphene-like molecules in the kilo-Dalton scale.

Keywords: compression, eigensolving, graphene, sensing, benzene, coronene



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A PEO@FE-DOPED ZIF-8 INCORPORATION FOR ENHANCING LITHIUM-ION TRANSPORT IN ALL-SOLID-STATE POLYMER BATTERIES

Ilhyeon Cho^a, Gyungmin Hwang^b, Seungjin Lee^a, Suyeon Kim^a, Daewon Chung^a,
Joonhyeon Jeon^{a,b,*}

^aDepartment of Advanced Battery Convergence Engineering, Dongguk University-Seoul, Korea

^bDivision of Electronics & Electrical Engineering, Dongguk University-Seoul, Korea

*Corresponding author: memory@dgu.edu

Abstract

The development of high-performance solid-state electrolytes remains a critical challenge for advancing all-solid-state batteries (ASSBs). While polymer electrolytes offer advantages in excellent interfacial contact with electrodes and cost-effective processing, their relatively low ionic conductivity and lithium-ion selectivity limit practical applications. This study introduces a novel strategy to enhance lithium-ion transport by developing a polymer electrolyte through incorporating 6 mol% Fe-doped ZIF-8 (FZ-6) into poly(ethylene oxide) (PEO) matrix. FZ-6 was synthesized with a controlled amount of Fe²⁺ ions was introduced during the ZIF-8 formation. The PEO@FZ-6 electrolyte was prepared by a solution casting method, where PEO and lithium bis(trifluoromethane-sulfonyl)imide (LiTFSI) were dissolved in acetonitrile (EO:Li=20:1), followed by the addition of 5 wt% FZ-6 and subsequent solvent removal. PEO@FZ-6 demonstrates superior electrochemical performance with ionic conductivity of $7.0 \times 10^{-4} \text{ S}\cdot\text{cm}^{-1}$ at 60 °C and lithium-ion transference number of 0.410, 2.1 times higher than that of conventional PEO-LiTFSI electrolyte.¹ The improved properties result from the expansion of Lewis acid sites within the FZ-6 structure, reinforcing Lewis acid-base interactions with TFSI⁻ anions. Consequently, the Li/PEO@FZ-6/Li symmetric cell demonstrates stable overpotential for over 1,000 hours during lithium stripping/plating tests. The enhanced interaction between FZ-6 and TFSI⁻ anions immobilizes anions, improving lithium-ion transport and suppressing lithium dendrite formation at the lithium metal interface by mitigating concentration polarization. Furthermore, PEO@FZ-6 assembled in a full cell configuration with LiFePO₄ cathode and lithium metal anode shows stable cycling at 60 °C and 0.1 C. This work presents a promising solution for developing high-performance polymer electrolytes through Fe-doped metal-organic framework strategy.

Acknowledgments This work was supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP), and the Ministry of Trade, Industry & Energy (MOTIE) of the Republic of Korea (No. 20224000000020).

Keywords: All-solid-state batteries (ASSBs), Polymer electrolyte, Fe-doped ZIF-8, Lewis acid-base interaction, Lithium-ion transference number

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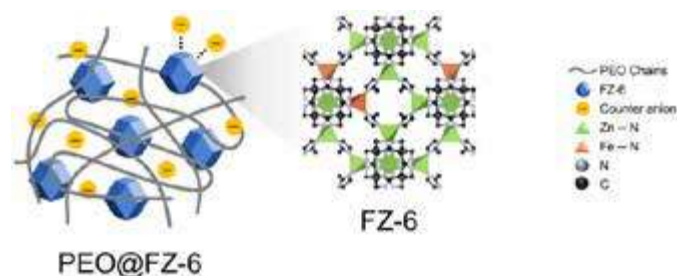


Figure 1 Schematic illustration of PEO@FZ-6 composite electrolyte and crystal structure of Fe-doped ZIF-8.

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HIGHLY DURABLE AND REVERSIBLE H_3PO_4 AND HNSO_3 MIXED ACID ADDITIVE FOR VANADIUM REDOX FLOW BATTERY ELECTROLYTE SOLUTIONS

Chaerin Yoon^a, Gyungmin Hwang^b, Deokhee Yun^b, Joonhyeon Jeon^{a,b,*}

^a Department of Advanced Battery Convergence Engineering, Dongguk University-Seoul, Korea

^b Division of Electronics & Electrical Engineering, Dongguk University-Seoul, Korea

*corresponding author: memory@dgu.edu

Abstract

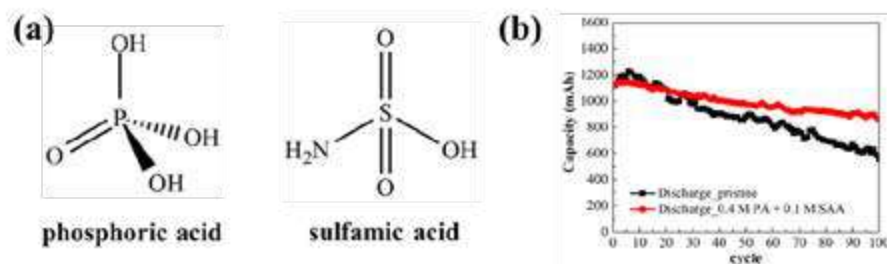
With the increasing global demand for electricity and the renewable energy sources implementation, vanadium redox flow batteries (VRFBs) have gained significant attention due to their scalability and enhanced flexibility. In this study, phosphoric acid (H_3PO_4) and sulfamic acid (H_2NSO_3) mixed acid additive was introduced to enhance the electrochemical performances. Various electrochemical property analyses were conducted to identify the effect of mixed acids as electrolyte additives to improve the performance of VRFBs. Cyclic voltammetry results revealed that the electrolyte with mixed acid additive exhibited favorable I_{pc}/I_{pa} ratio of 1.060 near unity and tight ΔE_p of 0.217 mV. These findings indicate that the V(IV)/V(V) redox reaction using the mixed acid additive system is more electrochemically reversible. Electrochemical impedance spectroscopy further demonstrated that electrolyte with the mixed acids additive exhibited the charge transfer resistance of 93.3 m Ω , suggesting enhanced vanadium ion and electron transport properties. Finally, electrolyte with the mixed additive was applied to a flow cell for charge-discharge performance evaluation. Results showed 95.30 % of Coulombic efficiency and 75.68 % of energy efficiency which is 0.18 and 2.97 % higher than pristine one. Also, retention ratio of the flow cell was 27.61 % higher than flow cell using electrolyte without additive during 100 cycles. This study highlights the potential of mixed acid additives to enhance the performance and stability of VRFBs, providing valuable insights for the development of high-performance energy storage systems.

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Keywords

Redox Flow Battery, Electrolyte, Mixed acid additive, phosphoric acid, sulfamic acid

Graphic/image (Optional)



(a) Structural formulas of two acid substances used as mixed acid additive. Sulfamic acid(left) and phosphoric acid(right).

(b) Capacity retention over 100 cycles for pristine and mixed acid additive cell.

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WEAK POLYELECTROLYTE MEMBRANES WITH A WIDE ION-EXCHANGE CAPACITY (IEC) RANGE AND LIMITED WATER SWELLING IN CLEAN TECHNOLOGIES FOR SUSTAINABILITY

Hee Jeung Oh^{a, b, c*}

^a Chemical Engineering, Pennsylvania State University, University Park, USA

^b Materials Science and Engineering, Pennsylvania State University, University Park, USA

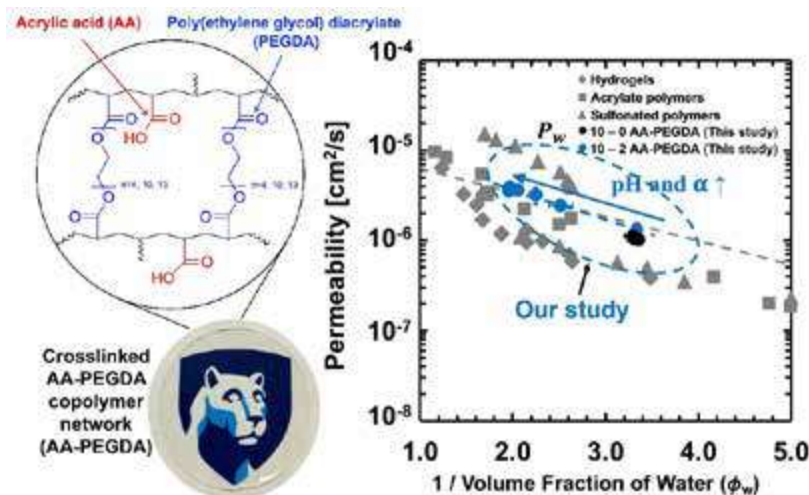
^c 2025 IUPAC Young Observer for the 53rd IUPAC General Assembly and 50th World Chemistry Congress the U.S. National Committee (USNC)

*Corresponding author: hjoh@psu.edu

Abstract

Charged polymer membranes are of great importance in membrane-based applications for environment, energy, and health due to their tunable transport properties. Designing innovative charged polymer membranes is thus required to advance clean technologies in sustainability. Here, we report on the design and characterization of a new library of weak polyelectrolyte membranes with a wide ion-exchange capacity (IEC) range and limited water swelling. This model system consists of a dissociable acrylic acid (AA) monomer and a poly(ethylene glycol) diacrylate (PEGDA) crosslinker. Specifically, using one fixed chemical structure, the charged group concentration (effective ion-exchange capacity) in the polymer can be systematically changed as a function of the external pH. This library offers a unique opportunity to study water and ion transport using the same chemical structure and thus helps us to establish a mechanistic understanding of ion transport in charged polymer membranes. We discuss water and ion transport properties including solubility, diffusivity and permeability in these materials and correlate the macroscopic transport properties with microscopic dielectric properties via dielectric relaxation spectroscopy. Our discussion can help to design the next generation of charged polymer membranes.

Keywords: Membrane, polyelectrolyte, charged polymer, ion-exchange capacity, transport



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THE STUDY OF POLYANILINE TERNARY NANOCOMPOSITE ON THE PHOTOCATALYTIC DEGRADATION OF TOXIC DYE

Wai-Leon Low^a, Chiam-Wen Liew^a, Joon-Ching Juan^b, Sook-Wai Phang^{a*}

^aDepartment of Physical Science, Faculty of Applied Sciences,
Tunku Abdul Rahman University of Management and Technology (TAR UMT),
Jalan Genting Klang, Setapak, 53300 Kuala Lumpur, Malaysia.

^bNanotechnology and Catalysis Research Centre, Institute for Advanced Studies, University of Malaya (UM),
50603 Kuala Lumpur, Malaysia

*Corresponding author: pinkyphang@gmail.com/ phangsw@tarc.edu.my

Abstract

The use of nanocomposites in the photocatalytic degradation of environmental pollutants has been proven effective in previous studies. In this research, ternary nanocomposites polyaniline – tin oxide – multiwalled carbon nanotube (PAni-SnO₂-MWCNT) with different weight percent of MWCNT were successfully synthesized using template free method. The chemical structures and oxidation states of the nanocomposites were confirmed by Fourier Transform Infrared (FTIR) and Ultra-violet visible (UV-Vis) spectroscopies respectively. The existence of SnO₂ was characterized by X-ray Diffraction (XRD) analysis while morphology of the nanocomposites was investigated by Field Emission Scanning Electron Microscopy (FESEM). Electrical conductivities of PAni-SnO₂-MWCNT were measured by conductivity meter showing conductivity range of $3.29 \times 10^{-3} - 4.42 \times 10^{-2} \text{ S cm}^{-1}$. The photodegradation performance of PAni-SnO₂-MWCNT for toxic RB5 dye was in the range of 60.65% - 94.12% in which PAni-SnO₂-MWCNT(20%) demonstrates the highest photocatalytic degradation efficiency of 94.12%. This is explained by the unique physical and optical properties of the nanocomposites attributed to the synergistic effect between PAni, SnO₂ and MWCNT.

Keywords: Polyaniline, tin oxide, MWCNT, ternary nanocomposites, photocatalytic degradation

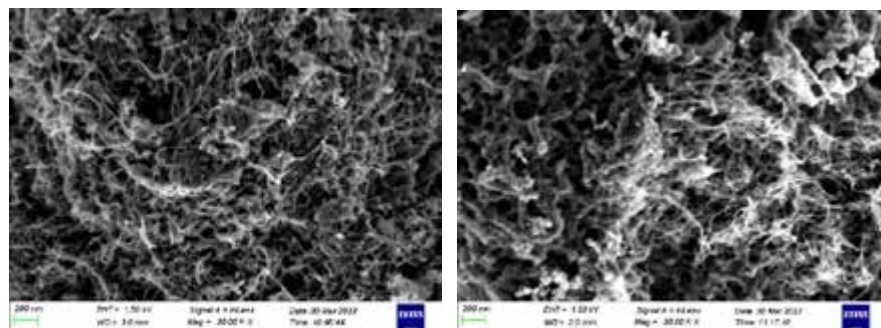


Figure 1: FESEM images of (a) PAni-MWCNT and (b) PAni-SnO₂-MWCNT (20%) with magnification of 30,000 $\times$.

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DESIGN AND FABRICATION OF HIGH-BARRIER PBAT FILMS BASED ON SELF-DRIVEN LAYERED DESIGN

Jing Yuan^a, Xinpeng Zhang^a, Jun Xu^a, Baohua Guo^{a*}

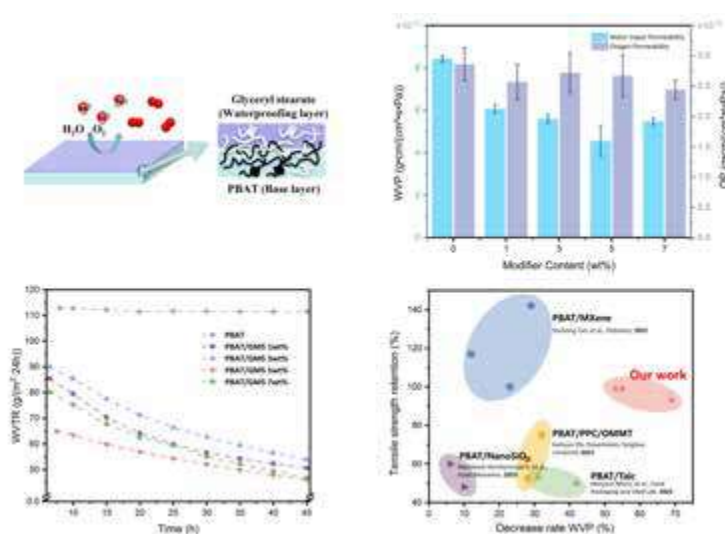
^aTsinghua University

*Corresponding author: bhguo@mail.tsinghua.edu.cn

Abstract

Biodegradable plastics have gained significant attention as potential alternatives to traditional polyolefin plastics, especially in packaging applications. Poly(butylene adipate-co-terephthalate) (PBAT) is a promising candidate due to its cost-effectiveness and excellent processing properties, but its poor barrier performance limits its applications. This study aims to enhance the water vapor barrier properties of PBAT by using self-driven layered design approach^{1,2}. Glycerol stearates, selected by molecular dynamics simulations, were incorporated into PBAT at varying concentrations, which are expected to spontaneously form a hydrophobic surface³. This surface modification significantly reduces the polarity of the PBAT, thereby enhancing its water vapor barrier performance. The results revealed an optimal water vapor permeability of 2.63×10^{-13} g·cm/(cm²·s·Pa), which are substantially lower than the permeability, 8.43×10^{-13} g·cm/(cm²·s·Pa), of neat PBAT. The water vapor permeability of the system was also proven to be time-dependent, which was attributed to the equilibrium and migration of the small molecules within the polymer matrix. Moreover, the incorporation of small molecules did not largely sacrifice its mechanical strength, indicating the potential for its application in biodegradable packaging materials.

Keywords: Biodegradable plastics, poly(butylene adipate-co-terephthalate), water vapor barrier properties, self-driven layered design, hydrophobic surface



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3D-PRINTABLE ALGINATE AND GRAPHITIC CARBON NITRIDE HYDROGEL FOR EFFICIENT SOLAR PHOTOCATALYTIC WATER SPLITTING

Khoiria Nur Atika Putri^a, Varol Intasanta^b, Autchara Pangon^c, Makoto Ogawa^d Voravee P. Hoven^{a*}

^a*Program of Petrochemistry and Polymer Science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand 10330*

^b*Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand 10330*

^c*National Nanotechnology Center, National Science and Technology Development Agency, Pathum Thani, Thailand 12120*

^d*School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Rayong, Thailand 21210*

*Corresponding author: vipavee.p@chula.ac.th

Abstract

As the world races through the carbon-neutral future, hydrogen (H₂) has emerged as a pivotal element in the global transition to clean energy with solar-driven photocatalysis standing out as a promising avenue. Graphitic carbon nitride (g-CN) as a metal-free photocatalyst offers an excellent visible light photocatalytic activity to enable photocatalytic solar water splitting, yielding H₂ but suffers from rapid charge recombination and practical efficiency in its particulate form. Herein, Platinum (Pt) deposition through a green photoreduction method was performed to increase the charge transfer efficiency in melamine-derived g-CN, resulting in a 20-fold increment in the amount of evolved H₂ under solar-simulated irradiation. Furthermore, to overcome practical use limitations, a 3D-printable bio-based hydrogel matrix derived from alginate was introduced to immobilize Pt-modified g-CN (Pt@g-CN) particles via hydrogen bonds. Exploiting the alginate hydrogel's unique physical properties that provide a hydrated microenvironment and induce internal light scattering within its porous interior along with hydrogel's macrostructure optimization via direct-ink-writing (DIW) 3D printing that facilitates uniform light propagation and mass transfer throughout the bulk surface resulted in a three-fold increase in the evolved H₂ compared to free Pt@g-CN particles. The 3D-printed alginate/Pt@g-CN hydrogel also presented excellent photoredox stability for 15 h. These findings highlighted the advantageous proposed synergistic approach to obtain practical, scalable, and sustainable material for green H₂ conversion.

Keywords: 3D printing, hydrogel, alginate, graphitic carbon nitride, photocatalytic water splitting

ULTRAFAST CHARGE TRANSFER CASCADE IN A MIXED-DIMENSIONALITY HETEROSTRUCTURE

Alexis R. Myers^{a,*}, M. Alejandra Hermosilla-Palacios^a, Jeffrey L. Blackburn^a

^aNational Renewable Energy Laboratory

*Corresponding author: alexis.myers@nrel.gov

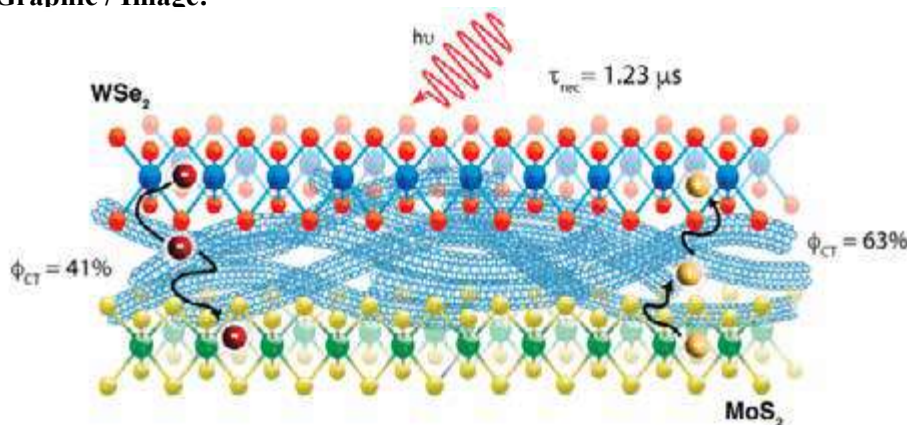
Abstract

Successful solar harvesting in optoelectronic semiconductor materials relies on a delicate balance between charge generation, charge extraction, and charge recombination. Despite recent advances, comprehensive mechanistic insights into charge transfer dynamics in low-dimensional materials remain limited. Using transient absorption spectroscopy, we investigate charge transfer and diffusion in a mixed-dimensionality MoS₂/SWCNT/WSe₂ heterotrilaier, where exciton dissociation at the MoS₂/SWCNT interface leads to charge separation and diffusion to the WSe₂ interface. This behavior contrasts with the strong Coulomb-bound interlayer excitons typically observed in TMDC heterostructures, highlighting the distinct photophysics and technological potential of mixed-dimensional systems.

A major challenge in nanoscale materials is the precise quantification of charge carrier densities, which introduces uncertainties in carrier density-dependent processes. Building on this work, we employ steady-state and transient absorption spectroscopies to establish a quantitative relationship between charge density, local dielectric environment, and excitonic properties. This approach provides a framework for estimating both ground- and excited-state carrier densities in TMDC-based systems, offering valuable insights into charge transport mechanisms and guiding the development of next-generation optoelectronic devices.

Keywords: Transition metal dichalcogenides, charge transfer, carbon nanotubes, heterostructures, transient absorption spectroscopy

Graphic / Image:



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UNCONVENTIONAL APPLICATIONS AND POTENTIALS OF BULK GRAPHENE MATERIALS

Tengfei Zhang^{a,*}

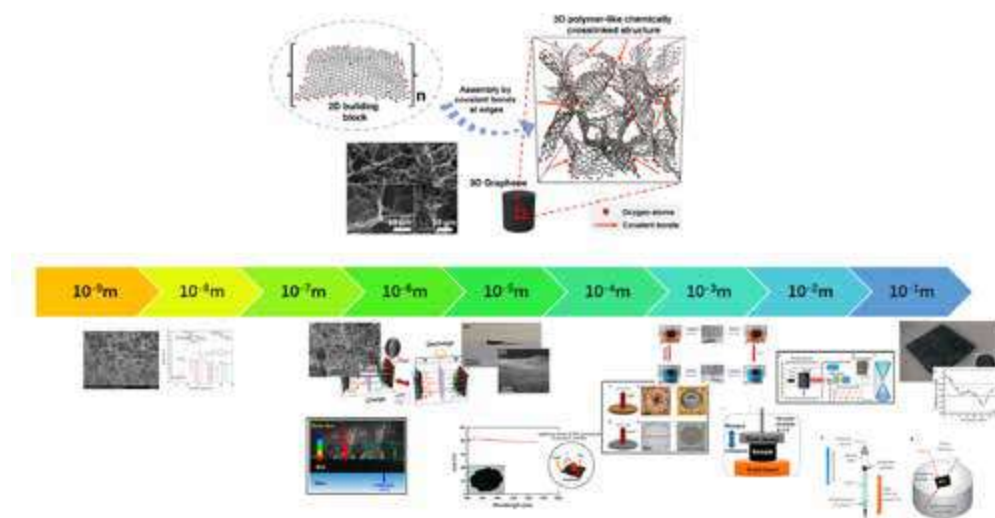
^aZhengzhou University

*Corresponding author: tengfeizhang@zzu.edu.cn

Abstract

Two decades have passed since the discovery of graphene in a strictly academic sense. The list of graphene's remarkable properties continues to expand extensively. Based on them, some applications have already been commercialized, although not reached their explosive growth stage yet. We believe that one of the primary scientific challenges in current graphene's research and application is to achieve macroscopic bulk graphene materials while preserving the intrinsic two-dimensional structure and characteristics of independent and individual graphene sheets. Here, I will succinctly review significant milestones in bulk graphene material research, with a particular focus on pure (not composite) bulk graphene materials. Additionally, I will highlight our investigations and endeavours related to bulk graphene materials and their unconventional applications. These include unrepresented properties or phenomenon in areas such as unconventional catalysis, light-matter interactions, and mechanical behaviours at extreme temperatures. Finally, I will briefly discuss potential avenues for future research on the application of bulk graphene in fields like near-space vehicles and low-temperature chemistry.

Keywords: graphene, bulk graphene materials, unconventional properties and applications, future potentials



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TANNIC ACID-GRAFTED POLYLACTIC ACID FILMS: A NONMIGRATING ANTIBACTERIAL PACKAGING FOR CHILLED FRESH MEAT

Linze Liu^a, Tungalag Dong^a, Xueyan Yun^{a*}

^a College of Food Science and Engineering, Inner Mongolia Agricultural University

*Corresponding author: yun_imau@163.com

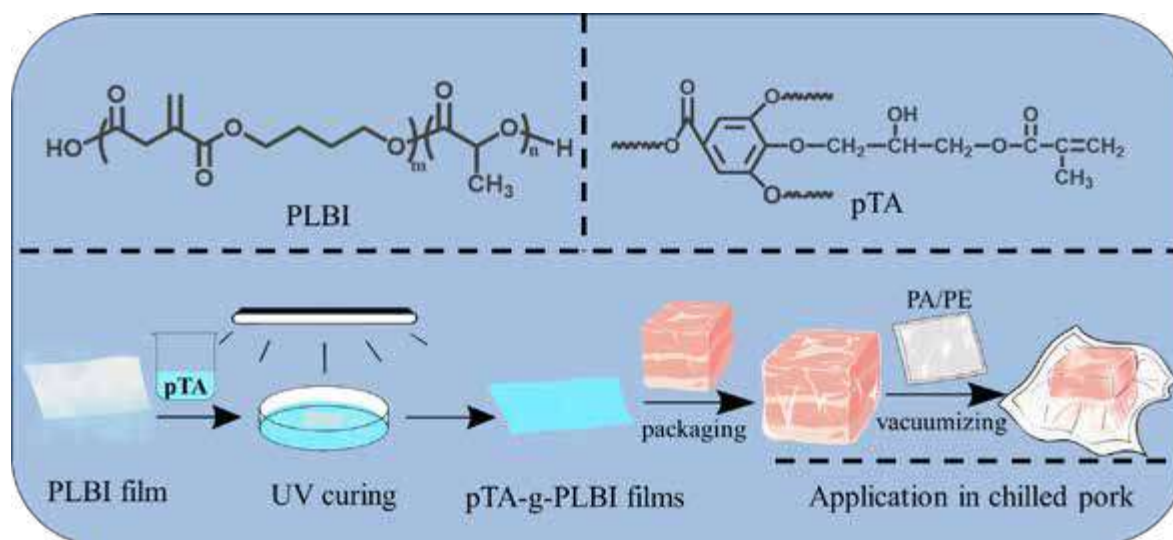
Abstract

Antimicrobial packaging can prolong the shelf life of fresh food, but those active antimicrobial substances may leach into the food and affect its quality. To avoid this phenome, the C—C double bond was first incorporated into the chemical structure of polylactic acid (PLLA) and tannic acid (TA) to prepare poly(L-LA-co-butyrate itaconate) (PLBI) and photoactive tannic acid (pTA). Then pTA-grafted PLBI (pTA-g-PLBI) films were fabricated using UV curing technology. Herein discussion will be focused on the following points with the goal of preparing nonmigrating antibacterial packaging for chilled fresh meat.

1. TA grafted on the surface of PLLA films (pTA-g-PLBI) using UV curing technology.
2. pTA-g-PLBI films inhibited the growth of *S. aureus*, *E. coli*, and *P. fluorescens*.
3. pTA-g-PLBI films extend the shelf life of chilled pork.
4. pTA-g-PLBI films changed the microbial diversity in chilled pork during storage.

As a result, The pTA-g-PLBI films exhibited good bacteriostatic effects of 86 %, 90 %, and 96 % on *E. coli*, *P. fluorescens*, and *S. aureus*, respectively. Additionally, pTA-g-PLBI packaging reduced the relative abundance of *Shewanella*, *Psychrobacter*, and *Pseudomonas* in chilled pork and delayed the deterioration of pork for more than 5 days.

Keywords: Tannic acid; PLLA; Grafted film; Antibacterial packaging; Chilled fresh meat



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PROTEIN SEPARATION USING CHITIN MONOLITH IN THE CONTINUOUS FLOW SYSTEM

Armeida D R Madjid^a, Hikaru Matsumoto^a, Yoshinori Kawabe^a, Masanori Nagao^a,
Yoshiko Miura^{a*},

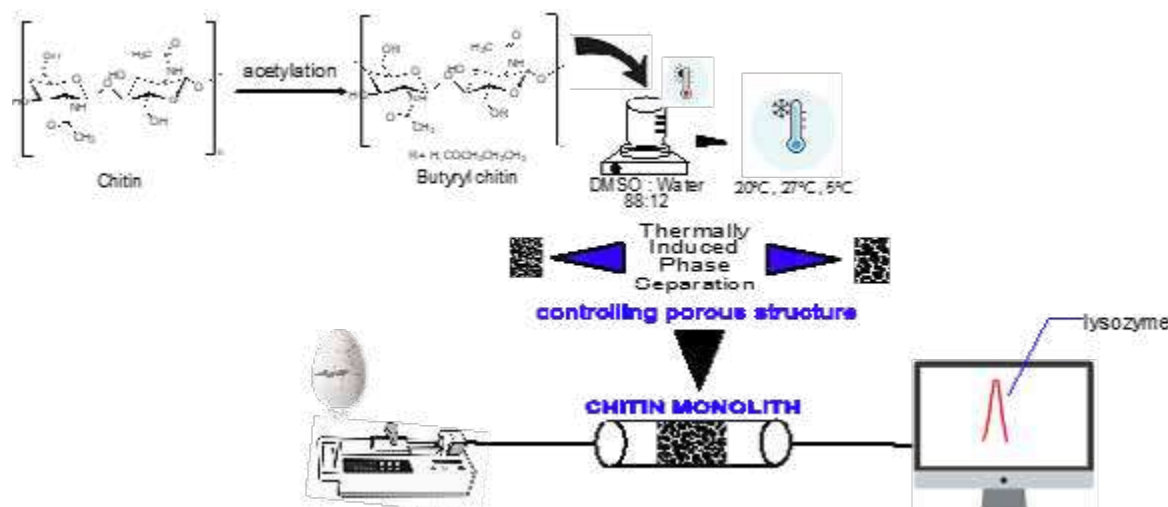
^aDepartment of Chemical Engineering, Graduate School of Engineering,
Kyushu University, 744 Motoooka,
Nishi-ku, Fukuoka 819-0395, Japan

*Corresponding author: miuray@chem-eng.kyushu-u.ac.jp

Abstract

Chitin, the second most abundant biomaterial after cellulose, is valued for its biocompatibility and eco-friendliness, making it ideal for biomedical applications. This study explores chitin monoliths, created via Thermally Induced Phase Separation (TIPS)¹, for protein separation in the continuous flow systems. The monoliths were prepared by modifying chitin into butyryl chitin (BC) and then hydrolyzing it to restore chitin's properties. Characterization using FE-SEM, FT-IR, and mercury intrusion porosimetry revealed tunable pore structures based on quenched temperatures. The monoliths showed high permeability and lysozyme affinity, with a flow system adsorption capacity of 107.5 mg/g, outperforming batch mode (86.2 mg/g). The 5 °C quenched monolith achieved the highest lysozyme-ovalbumin separation efficiency and effectively processed artificial samples and diluted egg white. The system demonstrated stability over multiple cycles with minimal capacity loss and improved leakage and dispersion issues compared to prior systems². This study highlights chitin monoliths as a sustainable and efficient tool for continuous protein separation, surpassing traditional batch methods.

Keywords: Chitin, monolith, protein, flow system, phase separation



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NITROGEN-SULFUR CO-FUNCTIONALIZED REDUCED GRAPHENE OXIDE FOR SUPERCAPACITORS: A PRELIMINARY STUDY

Raphael Guan Yuan Dino^a, Soon-Poh Lee^b, Omar Faruqi Marzuki^a, Alvin Teik Zheng Lim^{a,d}, Kwok Feng Chong^c, Ellie Yi Lih Teo^{a,d*},

^a*Department of Science and Technology, Faculty of Humanities, Management and Science, Universiti Putra Malaysia, Jalan Nyabau, 97008 Bintulu, Sarawak, Malaysia.*

^b*Lee Kong Chian Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, 43000 Kajang, Selangor, Malaysia.*

^c*Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang Sultan Al-Abdullah, Lebuhraya Tun Razak, 26300 Kuantan, Pahang, Malaysia.*

^d*Institute of Ecosystem Science Borneo, Universiti Putra Malaysia, Jalan Nyabau, 97008 Bintulu, Sarawak, Malaysia.*

*Corresponding author: ellie_teo@upm.edu.my

Abstract

Functionalization is a widely popular method used to overcome the drawbacks of graphene and enhance the performance of graphene in supercapacitors. In this work, we report on the physicochemical and electrochemical properties of nitrogen-sulfur co-functionalized reduced graphene oxide (N,S-rGO) for its suitability as a supercapacitor electrode. rGO was prepared via the modified Hummers' method and chemical reduction. rGO was subsequently co-functionalized with nitrogen and sulfur using ammonium persulfate (APS) as the functionalization agent. FTIR, UV-Vis and EDX analyses confirm the successful co-functionalization of nitrogen and sulfur on the N,S-rGO. The electrochemical properties of N,S-rGO was studied using cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD). N,S-rGO demonstrated substantial increase in the specific capacitance for N,S-rGO (381 F g^{-1} at 0.2 A g^{-1}) as compared to non-functionalized rGO (84 F g^{-1} at 0.2 A g^{-1}). The enhanced specific capacitance is attributed to the contribution of pseudocapacitance from nitrogen and sulfur as well as the synergistic effects of nitrogen and sulfur. This shows that the N,S-rGO is a potential promising electrode material for supercapacitors.

Keywords: nitrogen, sulfur, co-functionalization, reduced graphene oxide, supercapacitor

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INTEGRATED POTASSIUM HYDROXIDE-BASED BIOREFINERY FOR RICE STRAW: PULP PRODUCTION, LIGNIN RECOVERY, AND SPENT LIQUOR UTILIZATION IN AGRICULTURE

Razia Sultana Popy, and M. Mostafizur Rahman, M. Sarwar Jahan*,

Pulp and Paper Research Division, Bangladesh Council of Scientific and Industrial Research Laboratories, Dhaka, Dr. Qudrat-i-Khuda Road, Dhaka 1205, Bangladesh

Corresponding author: sarwar2065@hotmail.com

Abstract

Rice straw, a major agricultural residue in Bangladesh, offers a promising alternative fibrous raw material for a country with limited forest resources. However, its high silica content makes it unsuitable for conventional pulping processes. To address this, potassium hydroxide (KOH) pulping under mild conditions was investigated for producing packaging paper, while the spent liquor was evaluated for potential use as fertilizer. Under optimized conditions—8% KOH, 2 hours of cooking at 150°C, and a material-to-liquor ratio of 1:6—a pulp yield of 51% with a kappa number of 23.4 was achieved. The papermaking properties of the KOH pulp were found to be acceptable, and its tear strength was further enhanced by blending with bamboo pulp, making it suitable for kraft liner applications.

A portion of the lignin in rice straw was dissolved in the black liquor and subsequently precipitated by adjusting the pH to 7.38, 5.5, and 3.25 using dilute sulfuric acid. The spent liquor, rich in beneficial elements, was applied as a soil amendment, improving soil properties and promoting the growth of *Red amaranthus* and Kolmi sag in pot experiments. The isolated lignin from the KOH spent liquor exhibited lower methoxyl content, higher phenolic hydroxyl content, and lower molecular weight, making it a viable candidate to replace up to 40% of phenol in phenol-formaldehyde resin production.

Keywords: Pulp yield, Papermaking properties, Lignin, Fertilizer

SOLID-PHASE ELECTROSYNTHESIS

Mao Li

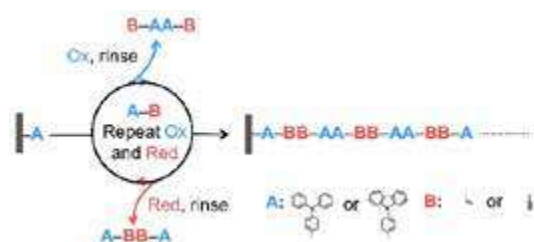
State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University,
Changchun 130012, China
*Limao@jlu.edu.cn

Abstract

The solid-phase synthesis developed by Merrifield in 1964 is widely employed for the synthesis of biological molecules, such as peptides, nucleic acids, and oligosaccharides. Generally, unsatisfied reaction dynamics at the solid-liquid interface cannot statistically permit accurate and uniform polymer synthesis of sophisticated structures and functions within an acceptable time scale.

We propose the concept of solid-phase electrosynthesis, which simultaneously enables rapid surface-initiated uniform electrosynthesis and unidirectional assembly of metallopolymer via kinetically accelerated and statistically allowed iterative growth. In particular, on a self-assembled monolayer (SAM) of the metal complex with electroactive unit A, the iterative monomer with two electroactive units A and B can be alternatively activated by oxidative and reductive potentials for A–A and B–B covalent couplings with the SAM, respectively. This enables topochemical one-by-one additions of the iterative monomers to end-on-oriented self-assembled molecules through alternative redox reactions. Each iterative step is purified by washing. Repeating the same iterative reaction enables further reaction of the unreactive sites on the SAMs and repairs the morphology defects, thereby ensuring the statistically allowed uniform synthesis and fabrication of polymer monolayers. The resulting monolayers exhibit subnanometer-uniform morphology over centimeter-sized areas with crystalline states and show thicknesses similar to theoretical molecular lengths.

The length-controlled electrosynthesis of metallopolymer can be generalized for many types of organic ligands and metal species, enabling quantitative design of the composition and sequence-controlled metallopolymer with the precise relationships of structures and properties. Through the utilization of precise and efficient iterative growth, this predictable electrosynthesis, coupled with optical and electrical monitoring, not only expands the scope of current synthetic chemistry but also paves a potential way for the automated generation of optoelectric molecular monolayers with large-area dimensional consistency and enhanced physical performance.



Keywords: solid-phase synthesis, solid-phase electrosynthesis, metallopolymer, polymer brush, polymer monolayer

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MOTILITY-INDUCED ORGANIZATION OF POLYMERS FROM ACTIVE MONOMER UNITS

Alexander Buglakov^{a,b}, Vasilisa Lelecova^{c,b}, Alexey Gavrilov^{c,b} and
Alexander Chertovich^{c,b,*},

^a *Semenov Federal Research Center for Chemical Physics, Moscow, Russia*

^b *INEOS RAS, Moscow, Russia*

^c *Lomonosov Moscow State University, Russia*

*Corresponding author: chertov@chph.ras.ru

Abstract

Active matter is a new and rapidly growing topic that describes systems with active agents that are capable to transform the surrounding's energy into their own. In such systems there is no classical thermodynamic equilibrium and unusual effects of self-ordering and segregation can be observed [1]. Such systems can be found on different spatial and temporal scales, ranging from bacteria and molecular motors to flocks of birds and fish swarms. But what happens if the active agents form polymer chains? Polymers are poor in entropy, and therefore more prone to self-ordering and structurization than low-molecular-weight systems. Several models of polymers with active monomer units will be used to demonstrate their peculiarities and unusual properties, including their ability to undergo co-directed collective motion [2], collapse under the influence of activity [3], and even microphase separation. In addition to possible future technological applications, we believe that these kinds of interactions may play a key role in structuring DNA in eukaryotic nuclei, including the separation into eu- and heterochromatin. This work was financially supported by the RSCF (project 23-73-0008).

Keywords: Active matter, polymer collapse, copolymer

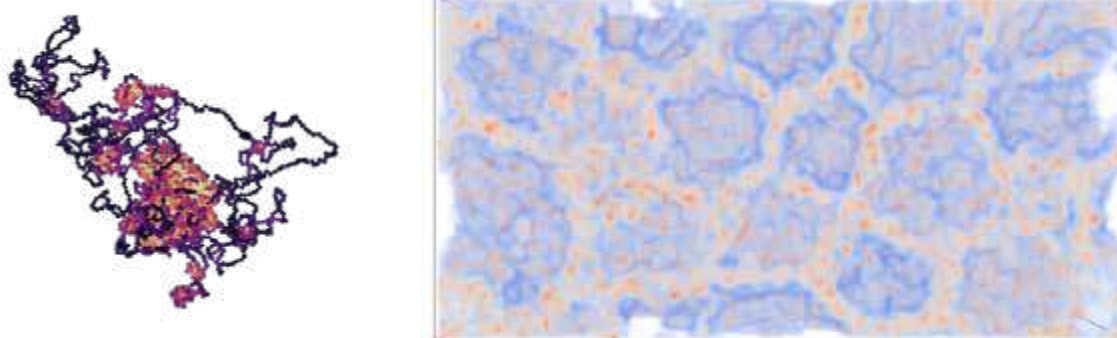


Figure 1. Example of polymer system with active monomer units as a single chain (left) and unusual microphase separation in a concentrated solution (right).

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PRE-VULCANIZATION EFFECTS ON COMPOUNDING, MATURATION, THERMAL STABILITY, AND MECHANICAL PROPERTIES OF EPOXIDIZED NATURAL RUBBER LATEX-CITRIC ACID (ENR-CA) FILMS

Anis Abdul Ghani^a, Fatin Nurshahirah Shahabuddin^a, Nafeesa Mohd Kanafi^a, Azira Abd Aziz^b,
Norizah Abdul Rahman^{a,c*}

^aDepartment of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia.

^bScience and Technology Latex Unit, Technology & Engineering Division, Stesen Penyelidikan RRIM, LGM 47000 Sungai Buloh, Selangor, Malaysia.

^cLaboratory of Nanomaterials Processing and Technology, Institute of Nanoscience and Nanotechnology, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

*Corresponding author: a_norizah@upm.edu.my

Abstract

This study explores the use of citric acid (CA) and sulfur (S) as vulcanizing agents in preparing pre-vulcanized epoxidized natural rubber/citric acid/sulfur (ENR/CA/S) blend films. The research focuses on the pre-vulcanization process over different compounding times and maturation periods, aiming to achieve full maturity within 24 hours. Results indicate that the total swelling index (TSI) decreased from 1.70 at 72 hours to 24 hours of maturation when compounded for 4 hours. ENR/CA/S films with 5–10 phr CA exhibited a reduction in TSI as sulfur content increased, accompanied by longer compounding times and greater crosslinking density. The effects of CA and sulfur content on the thermal and mechanical properties of the optimized pre-vulcanized ENR/CA/S were also investigated. The films were characterized for tensile strength (TS), elongation at break (EAT), and tensile modulus. The results showed that increasing CA content from 5 to 10 phr reduced the pH while slightly enhancing crosslinking density and mechanical strength. However, at 15 phr CA, mechanical properties declined significantly due to the denaturation of proteins within the rubber particles. Additionally, thermal stability decreased with higher CA content, suggesting a plasticization effect at elevated levels of CA. The pre-vulcanized ENR/5CA/0.9S formulation demonstrated optimal thermal and tensile properties, achieving a glass transition temperature of -21.77°C and a tensile strength of 4.18 MPa. This formulation shows potential for application in various latex-dipped products, including gloves, balloons, condoms, and medical tubing.

Keywords: Self-healing rubber, natural rubber, citric acid, epoxidized natural rubber, rubber composite

SOLID SUPPORTED IMIDAZOLIUM BASED ON NATURALLY OCCURRING BIOPOLYMER, SPOROPOLLENIN.

Kumuthini Chandrasekaram^{a,*}, Sharifah Mohamad^b, Yatimah Alias^{b,c}

^aHigher Institution Centre of Excellence (HICoE), UM Power Energy Dedicated Advanced Centre (UMPEDAC), Level 4, Wisma R&D, Universiti Malaya, Jalan Pantai Baharu, 59990 Kuala Lumpur, Malaysia.

^bDepartment of Chemistry, Faculty of Science, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.

^cFaculty of Industrial Sciences and Technology, Universiti Malaysia Pahang Al-Sultan Abdullah, Pahang, Malaysia.

*Corresponding author: kumuthinic@um.edu.my

Abstract

Sporopollenin is a natural biopolymer found in the outer membranes of moss, fern spores, and pollen grains. Sporopollenin has been referred to as the most resistant organic material of natural biological origin, and its robustness has resulted in a steady rise in interest. The potential of sporopollenin as an effective biosorbent has been observed in many recent reported works where modified sporopollenin has been applied as a targeted adsorbent for various analytes, including drugs, metals, dyes, and pesticides. This study attempts to tackle the challenge by functionalizing the surface with a series of imidazolium-based-ionic liquids, characterized and subsequently applied for targeted analyte absorption. Characterization techniques such as FTIR, solid-NMR, FESEM & EDX analysis while the analyte absorption study used spectroscopic methods. Methyl, butyl, decyl, and benzyl-imidazolium-based sporopollenin were successfully synthesized and characterized. The absorption of analytes was largely influenced by the type of imidazolium functionalization paving the way for imidazolium-functionalized sporopollenin to be used for targeted analyte adsorption.

Keywords: solid-supported ionic liquids; imidazolium; biopolymer; sporopollenin; surface modification

Graphic / Image



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RECYCLING POST-CONSUMER POLYPROPYLENE UTENSILS INTO 3D PRINTING FILAMENTS FOR FUSED FILAMENT FABRICATION

Chan Ming Yeng^{a,*}, Ong Shu Yong^a, Koay Seong Chun^b, Ho Shuh Huey^a

^aCentre for Advanced Materials, Faculty of Engineering and Technology, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Kelang, Setapak, 53300 Kuala Lumpur, Malaysia.

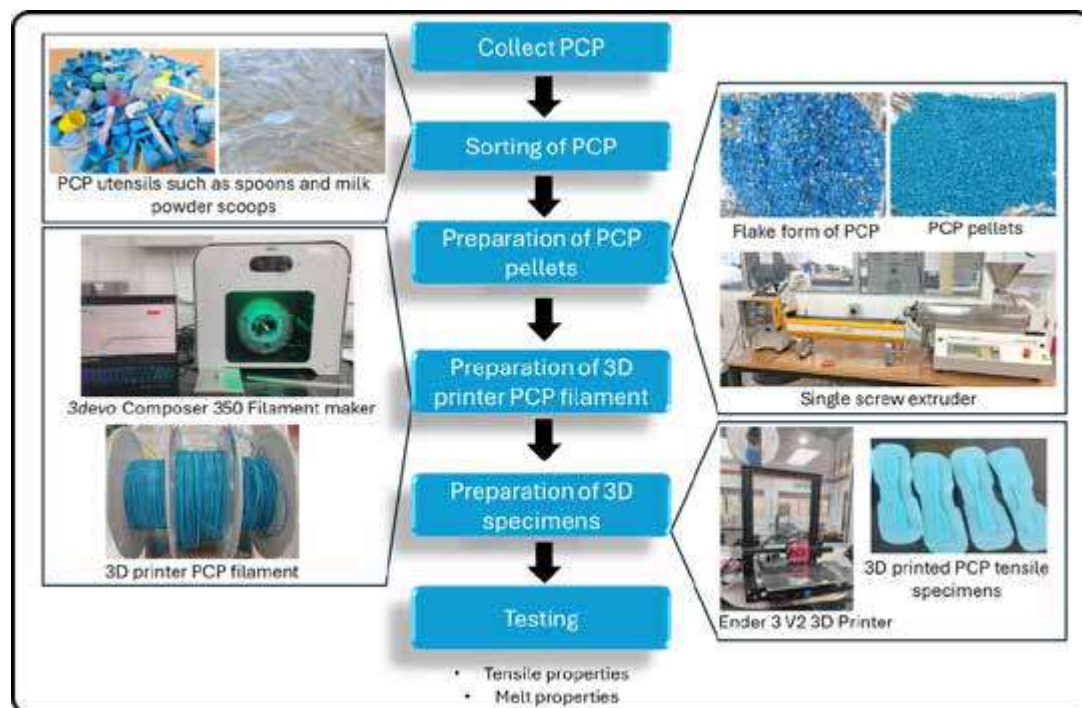
^bLee Kong Chian Faculty of Engineering and Science, Department of Mechanical and Materials Engineering, Universiti Tunku Abdul Rahman, Bandar Sungai Long, 43000 Kajang, Selangor, Malaysia.

*Corresponding author: chanmingyeng@taru.edu.my

Abstract

Plastic waste is the major issue causing the environmental pollution worldwide. The concern about the accumulation of plastic waste is increasing, and not everyone participates in plastic recycling, which leads to environmental problems. One of the solutions to addressing the plastic waste problem is to reuse and reduce plastic waste. The research study focuses on developing three-dimensional (3D) printer filament from post-consumer polypropylene (PCP), specifically from utensils such as spoons and milk powder scoops using single screw extruder and filament maker. Since PCP consists of both injection and extrusion grades of the polypropylene, the study aims to determine the suitable mixing ratio of these grades for filament production. A composition of 60 wt% injection-grade PCP mixed with 40 wt% extrusion-grade of PCP resulted in more uniform filament diameter compared to compositions with 50 wt% and 40 wt% extrusion-grade of the PCP. The melt flow index results also indicate that the addition of more extrusion-grade PCP causes a decrease in the melt flow rate, making the PCP mixture suitable for extrusion into 3D printing filament. The tensile strength of the printed specimens using PCP mixed filament exhibited approximately 30 MPa, and they were more ductile. Furthermore, this research proposes using post-consumer plastic in additive manufacturing as a sustainable alternative for virgin polymer. Additionally, this 3D printer filament can be used to produce non-load-bearing products such as architectural models, prototypes, decorative items, and more.

Keywords: 3D printer filament, recycled polymer, post-consumer utensils, tensile properties, fused filament fabrication.



NANOTABULAR STRUCTURES DISPLAYING HIGH HYDROPHOBICITY AND STRONG WATER ADHESION

Abdoulaye Dramé^a, Diawo Diallo^a, Hawa Ndiaye^a, Aminata Niang^a, Thierry Darmanin^b,
Frédéric Guittard^b

^aLaboratoire de Chimie Organique et bioorganique, Faculté des Sciences et Techniques Université Cheikh Anta Diop, BP 5005 Dakar, Sénégal

^bNICE Lab IMREDD 61-63 avenue Simone Veil 06100 Nice, Université Côte d'Azur

Abstract

Controlling structures at the nanoscale is a great of importance for a huge number of applications including, medical treatments, food packaging, and surface wetting properties [1-2]. Biomimicry of rose petals adhesion, allows the design of surface structures with the same properties [2]. In this context, original monomers were synthesized by grafting two thiophene or carbazole-based substituents onto naphthalene platform for its strong π stacking interactions. In the presentation, we study the effect of the position of the carbazole (ortho, meta, and para-positions) relative to other substituents during the electrodeposition process. Electropolymerization was performed by cyclic voltammetry and at constant potential. The results highlight highest level of hydrophobicity and strong water adhesion, of surfaces with nanotubes and nanoparticles, depending of the increase in conjugation length. These new materials have many domestic and industrial applications related to their special surface properties.

Keywords: Conjugated Monomers, Electropolymerization, Nanotubes, High Hydrophobicity, Strong Water Adhesion.

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INTERCONNECTIVITY OF MICROCELLULAR FOAMS PRODUCED VIA HIGH INTERNAL PHASE EMULSION TEMPLATING

Reza Foudazi^{a,*}, Muchu Zhou^a

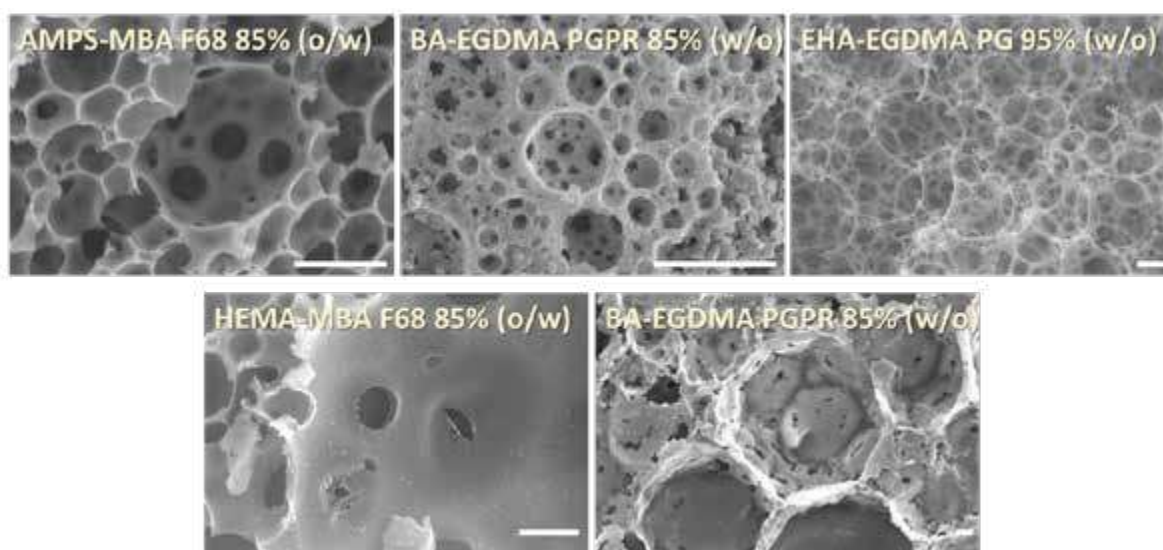
^a School of Sustainable Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, OK 73019, USA.

*Corresponding author: rfoudazi@ou.edu

Abstract

High internal phase emulsions (HIPEs), also known as highly concentrated emulsions (HCEs), are usually defined as emulsions with volume fraction higher than 0.74. PolyHIPEs, which are in the class of microcellular foams, are produced by polymerizing the continuous phase of the HIPE and then extracting the dispersed phase. PolyHIPE systems have been used in several applications, such as membranes, hydrogels, scaffolds for tissue engineering and cell culture, and catalyst supports. PolyHIPEs have a complex morphology consisting of cavities (voids, also called as pores) originally occupied by the emulsion droplets. Also, interconnecting holes usually exist between neighboring voids, called windows or pore throats. The interconnectivity of polyHIPEs is controlled by pore throat size and frequency. In this talk, we will discuss the parameters that influence the interconnectivity of polyHIPEs. Specifically, we will discuss the effect of interdroplet interaction (affecting flattened area and interdroplet layer thickness between neighboring droplets as well as the interdroplet layer drainage), interfacial film strength, and droplet arrangement on window size and frequency.

Keywords: Porous Polymers, Drainage, Depletion attraction, Pickering emulsions, Yield stress.



SYNTHESIS AND DESIGN OF ANIONIC POLYMERS AND MICROGELS FOR BIOMEDICAL ADHESIVES

Elena Yu. Kozhunova^{a*}, Elizaveta K. Kuznetsova^a, Anna V. Plutalova^a, Vitaly S. Kravchenko^b, Elena V. Chernikova^a, Igor I. Potemkin^a

^a*M.V. Lomonosov Moscow State University, Moscow, Russia*

^b*INEOS RAS, Moscow, Russia*

**Corresponding author: kozhunova@polly.phys.msu.ru*

Abstract

Materials with high adhesion are widely used in many areas: in the fabrication of composite materials, the manufacture of paints and varnishes and glues, in various biomedical applications. For example, polymer-based medical adhesives are used to join tissues in cases of injuries and incisions. Such materials not only speed up the process of incision closure, but also reduce the risk of injury and the spread of infectious diseases. When choosing a composition, it is important to note that adhesives used in regenerative medicine must be biocompatible and have high adhesion without interfering with tissue growth. One way to solve this problem may be to use adhesives obtained by forming dynamic non-covalent bonds between components. In this work, a number of anionic water-soluble polymers of various compositions and structures were synthesized under radical polymerization conditions for long-term use as one of the components of medical adhesive. The following objects were obtained: a) linear polymers, b) branched polymers and c) microgels, which included hydrophilic, hydrophobic and anionic monomer units.

For the synthesis of linear and branched polymers, reversible chain transfer polymerization¹ was used in aqueous or organic media. Water-soluble copolymers of acrylic acid (AA) and N-isopropylacrylamide (NIPAM), sodium styrene sulfonate with NIPAM, and AA with styrene were obtained and characterized. Synthesis of microgels was carried out by the method of green polymerization in water. Microgels based on copolymers of NIPAM and AA, and NIPAM and sodium styrene sulfonate were obtained and characterized. Further, the methods of dynamic light scattering, X-ray scattering and rheology were used to study the features of the thermal and pH behavior of polymers in aqueous solutions to determine the optimal compositions for further inclusion in the composition of the adhesive. Comprehensive computer simulations were also performed to give the insight into the system's architecture influence on adhesive properties.

Keywords: polymer adhesives, polymer electrolytes, microgels, branched polymers, RAFT polymerization, computer simulations

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FREQUENCY-DEPENDENT ELECTRICAL CONDUCTIVITY OF POLYVINYLIDENE FLUORIDE NANOCOMPOSITES REINFORCED WITH CuO AND TiO₂

Labi Agrawal¹, Gautam Patel^{1*}

¹*Chemistry Department, Parul Institute of Applied Science, Parul University, Vadodara-391760, Gujarat, India.*
Corresponding author: labi.agrawal023@gmail.com

Abstract

This study investigates the electrical conductivity performance of polyvinylidene fluoride (PVDF) nanocomposite films incorporating copper oxide (CuO) and titanium dioxide (TiO₂) nanoparticles. The electrical conductivity of the nanocomposites increased significantly from 10⁻¹² S/m for pure PVDF to 10⁻⁵ S/m for optimized PVDF-CuO-TiO₂ compositions, demonstrating a seven-order magnitude enhancement. The percolation threshold was identified at approximately 4 wt% total filler loading, above which conductivity increased exponentially. Impedance spectroscopy confirmed the formation of conductive networks through the polymer matrix, with decreased charge transfer resistance in the CuO-TiO₂ hybrid systems compared to single-filler counterparts. X-ray diffraction (XRD) and scanning electron microscopy (SEM) analyses confirmed the successful incorporation and uniform dispersion of nanoparticles within the PVDF matrix. The synergistic effect of combining semiconducting CuO with dielectric TiO₂ significantly enhanced the electrical conductivity and dielectric properties of the nanocomposites, making these materials promising candidates for applications requiring tunable electrical properties in flexible, lightweight polymer films.

Keywords: Polymer nanocomposites, EMI Shielding, Electrical Conductivity, Flexible Electronics

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ENHANCING DIELECTRIC PROPERTIES OF POLY (VINYLIDENE FLUORIDE) NANOCOMPOSITE FILMS INCORPORATED WITH BaTiO₃ AND ZrO₂ NANOCOMPOSITES

Yash Ughade¹, Gautam Patel^{1*}, Nitin Shingne^{2*}

^{*1}Chemistry Department, Parul Institute of Applied Science, Parul University, Vadodara-391760, Gujarat, India.

^{*2}Electrical Research and Development Association (ERDA), ERDA road Makarpura, Vadodara-390010, Gujarat, India.

Corresponding author: yashughade639@gmail.com

Abstract

The novel tertiary nanocomposite films containing barium titanate (BaTiO₃) and zirconium dioxide (ZrO₂) as nanofillers incorporated within polyvinylidene fluoride (PVDF) used as a polymer matrix is synthesized and analysed in this present report. Optimization of thermal and electrical properties is carried out by synthesizing the nanocomposites films with different concentrations of nanofillers using solution casting method. The confirmation of successful incorporation of both the nanofillers and enhancement of β -phase formation in PVDF, essential for piezoelectric properties are revealed by X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) analyses. Scanning Electron Microscopy (SEM) revealed the even distribution of nanofillers into the polymer framework with minimum accumulation. The dielectric analysis demonstrated a significant improvement in dielectric constant (ϵ') from pure PVDF to the prepared nanocomposite, also showing minimal dielectric loss in a broad range of frequency (10^1 to 10^7 Hz). The increment of thermal stability along with decomposition temperature increased by 42°C with respect to pristine PVDF is confirmed by thermal gravimetric analysis. These tertiary nanocomposite films serve as a promising choice for applications in flexible electronics, energy storage devices, and sensors technologies by being an excellent combination of high dielectric constant, enhanced mechanical flexibility and minimal dielectric loss.

Keywords: Polyvinylidene fluoride, nanocomposite films, dielectric properties, energy storage.

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HIGH-THROUGHPUT APPROACHES TO SUSTAINABLE MACROMOLECULAR ENGINEERING

Melody A. Morris^{a,*}, Alexandra Grinevich^a

^aDepartment of Polymer Science & Engineering, University of Massachusetts Amherst, Amherst, MA, USA.

**Corresponding author: melodymorris@umass.edu*

Abstract

Polymeric materials have become ubiquitous in modern life, both in everyday items, such as films for food storage, and in specialty applications like critical biomedical devices; moving to sustainable versions of each of these polymers to control their end-of-life responsibly is one of the greatest necessities of modern polymer science. Macromolecular samples are inherently complex and characterized by their chemistry, molecular weight distribution, monomer segment distribution, and architecture; together, the local design dictates the macroscopic and microscopic properties of the polymer of interest. To gain understanding and design rules for these complicated macromolecules, it is essential to move toward more high-throughput data generation and data-driven learning to probe how molecular design affect key physical properties. Protein-based systems are traditionally much more controlled, as each protein can be produced with perfect sequence definition, allowing for highly ordered intramolecular structures. Bringing together the complexity of polymer-based systems with the well-developed biosynthetic toolbox will allow for progress in both areas. This talk will focus on the development of high-throughput tools to generate sustainable protein- and polymer-based materials, which can be rapidly tested and iterated to affect a number of application spaces, spanning biomaterials, plastic recycling, and structural materials. A high-throughput pipeline for enzymatic polymer degradation will be demonstrated, using well-defined polymer substrates with controlled crystallinity and surface area, enabling data-driven learning for these complex systems. This research will promote first-of-its-kind comparison between different polymer substrates and enzyme types. By harnessing a combination of systematic materials design improvements, the connection of macroscopic properties and fundamental polymer physics principles will be realized with an end goal to systematically control polymer end-of-life.

Keywords: Enzymatic depolymerization, automation, high-throughput experimentation, sustainable polymers

OPTIMIZATION OF POLYLACTIDE SYNTHESIS USING FLOW CHEMISTRY

Glenn Clothier^a, Daniel Taton^a, Simon Harrisson^a

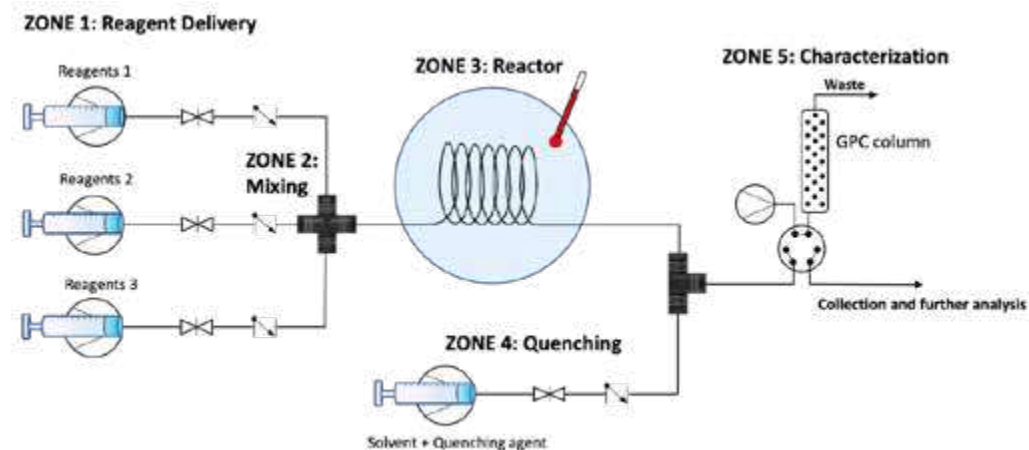
^aUniversity of Bordeaux – CNRS – Bordeaux INP, LCPO

*Corresponding author: sharrisson@enscbp.fr

Abstract

Increasing demand for sustainable polymers has driven research into degradable alternatives such as polylactide (PLA), a widely used aliphatic polyester known for its biocompatibility, crystallinity, and potential to replace commodity plastics. Despite its advantages, PLA faces challenges such as high production costs and slow degradation. Machine learning and automated chemistry are revolutionizing materials discovery, with continuous flow polymerization emerging as a promising method due to its improved control, scalability, and safety. Flow chemistry facilitates high-throughput synthesis, automated characterization, and real-time optimization.¹ While relatively few studies have explored the organocatalyzed ring-opening polymerization of lactide in flow systems, recent research has demonstrated its potential for enhanced control and efficiency.^{2,3} This study investigates PLA synthesis in a flow reactor, optimizing reaction conditions by varying residence time and catalyst concentration. Automated reagent addition and online characterization by size exclusion chromatography enable rapid generation of data, which is used to develop a non-parametric model of the reaction and identify Pareto-optimal reaction conditions maximizing both the overall conversion of lactide and the rate of polymer production. These conditions were subsequently validated experimentally in both flow and batch reactions.

Keywords: Polylactide, ring-opening polymerization, flow chemistry



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AIR-STABLE COVALENT ORGANIC FRAMEWORKS AS MULTIFUNCTIONAL LUBRICANT ADDITIVES

Ahmad Nasri Mohd Shafie^{ab*}, Novina Malviya^b, Maria Teresa Sateriale^c, Fergal Coleman^b, Suhaimi Abdul Razak^a, Andrea Dolfi^c, Geetha Srinivasan^a, Stuart James^b, Malgorzata Swadzba-Kwasny^{b*}

^aPETRONAS Research Sdn Bhd (PRSB) Malaysia

^bThe QUILL Research Centre, School of Chemistry and Chemical Engineering, Queen's University Belfast, UK.

^cPETRONAS Global Research & Technology Centre, Santena, Turin, Italy

*Corresponding author: nasri_shafie@petronas.com, m.swadzba-kwasny@qub.ac.uk

Abstract

Two-dimensional covalent organic frameworks (2D COFs) are an emerging class of crystalline, lightweight, porous, and tunable functional materials, composed of second-row elements (B, C, N, O).¹ Inherently free of metals, sulfur and phosphorus, all of which are potential poisons for catalytic converters,² COFs make attractive candidates as sustainable lubricant additives. In this study, air-stable boroxine-linked COFs (COF-1 N008), stabilised with tetraethyl orthosilicate (TEOS) and amines, were synthesised and evaluated as multifunctional additives in Group III+ base oil (KV₁₀₀ = 4.13 cSt, VI = 132). Dispersion stability, assessed using a LUMiSizer analytical photo-centrifuge,³ showed a 27% enhancement upon addition of 0.2 wt% of a commercial surfactant, effectively mitigating particle agglomeration - an inherent limitation of dispersion-type additives. Tribological testing using a high-friction reciprocating rig (HFRR) at 0.1 wt% COF-1 N008 with 0.2 wt% stabiliser revealed a synergistic effect, achieving a 55% reduction in both friction and wear relative to the base oil. SEM-EDAX analysis of the HFRR wear track confirmed the presence of nitrogen from COF-1 N008, supporting its active tribological role.⁴ The tribological performance could be attributed to surface incommensurability between COF layers, resulting in low friction sliding motion as well as enhanced dispersibility of octylamine's extended alkyl chain.

Keywords: covalent organic framework, friction and anti-wear, lubricant additives, analytical centrifugation, dispersion stability

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STARCH MATERIALS: OPPORTUNITIES AND CHALLENGES

Long Yu*, Jun Fu, Yiwen Yang, Qingfei Duan,
Institute of Chemistry, Henan Academy of Sciences, China
*Corresponding author: felyu@scut.edu.cn

Abstract

The development and production of biodegradable materials from renewable resources have been spurred by oil shortages and the growing interest in easing the environmental burden of petro-chemically derived polymers. Currently more and more countries have introduced regulations and laws of banning disposable plastics. Starches offer a very attractive low-cost base for new biodegradable polymers due to their low material cost and ability to be processed with conventional plastic processing equipment. During the quick development of bio-based materials recently, starch-based materials face both challenges and opportunities. Various conventional processing techniques such as extrusion, injection compression molding, and casting, as well as some new techniques such as reactive extrusion, have been adapted for processing starch-based polymers. On other hand, the study of the unique microstructures of different starches and their multiphase transitions during thermal processing have increased fundamental knowledge of polymeric science, in particular to understand the structure–processing–property relationships in polymers. This presentation will introduce our achievements in developing starch-based materials, including both fundamental issues like gelatinization, phase transition, chemical and physical modifications and application challenges like weaker mechanical properties, moisture sensitivity and instability. Based on the natural behaviors and modifications of starches we have developed and commercialized various starch-based edible materials, including edible food packaging or materials used as animal feeders for post-products. For examples, edible film used for easy noodle packaging, medical capsules, various packaging trays and foams. Another promised application is starch foam materials, which have been used for various packaging. The new directions will be discussed based on our achievements and experience.

Keywords: Starch; materials; biodegradable; edible.

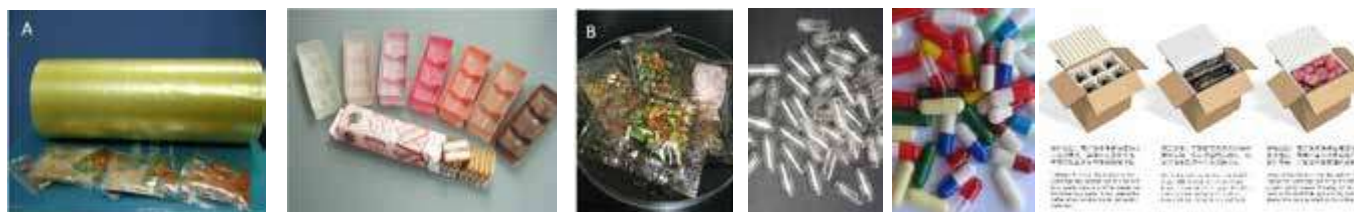


Figure 1. Photos of starch-based materials

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TAILORING MULTIPOROUS CARBON NANOMATERIALS VIA ELECTROSPUN POLYACRYLONITRILE BLOCK COPOLYMERS: EFFECTS OF COMPOSITION AND PROCESSING ON MORPHOLOGY AND POROSITY

Peter E. Mallon* and David Sibanda

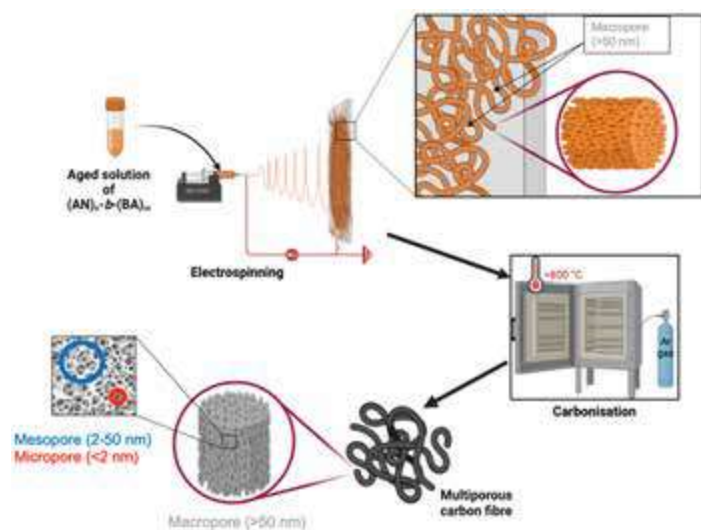
Department of Chemistry and Polymer Sciences, University of Stellenbosch, Stellenbosch, Private Bag X1, Matieland, 7602, South Africa.

**Corresponding author: pemallon@sun.ac.za*

Abstract

This study presents a method for producing multiporous carbon nanomaterials using high-molecular-weight polyacrylonitrile-*b*-poly(butyl acrylate) (PAN-*b*-PBA) block copolymers synthesised via atom transfer radical polymerization (ATRP). The precursors were processed into nanoparticles or nanofibers by electrospinning. The resulting multiporous structure arises from both the microscale morphology of the electrospun materials and the mesoporous architecture templated by the block copolymer, where the sacrificial degradation of the PBA segment during carbonization creates additional porosity. This study examines the effects of varying PAN and PBA block lengths, as well as processing parameters, particularly solution ageing, on fibre and particle morphology and porosity. High-molecular-weight PAN-Br is essential for obtaining a spinnable solution capable of forming nanofiber precursors, whereas low-molecular-weight precursors tend to form nanoparticles via electrospray. The results indicate that ageing the electrospinning solution increases the fibre diameter and transitions the structure from smooth-porous to rough-porous, likely due to physical crosslinking and intermolecular interactions in concentrated solutions. This transformation was also observed in films cast from the aged solutions. Additionally, a higher PBA content promotes phase separation, enhancing the porosity of both the precursor and carbonised fibres, and yielding materials with increased surface areas. This investigation highlights the critical role of the solution parameters and processing conditions in controlling the structure and properties of carbon nanofibers, offering insights into the tailored design of multi-porous carbon nanomaterials with specific morphologies.

Keywords: solution ageing; electrospinning; multi-porous carbon materials; porous, fibers



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FIRST-PRINCIPLES INVESTIGATION OF THE STRUCTURAL AND MECHANICAL PROPERTIES OF PtO₂/ALN VAN DER WAALS HETEROSTRUCTURES FOR POTENTIAL ANODE APPLICATIONS

Blessing F. Masora^a, Krishna K. Govender^a, Francis Opoku^b, and Penny. Govender^{a*},

^aDepartment of Chemical Sciences, University of Johannesburg, Johannesburg, South Africa

^bDepartment of Chemistry, Faculty of Physical and Computational Sciences, College of Science, Kwame Nkrumah University of Science and Technology, PMB, Kumasi, Ghana

*Penny Govender: pennyg@uj.ac.za

Abstract

The anode plays a vital role in the overall performance of a battery [1]. Recently, two-dimensional (2D) heterostructures have exhibited great potential as anode materials as a result of the combination of properties of different materials [2]. The structural and mechanical properties of PtO₂/AlN heterostructure were investigated using first-principles computational methods [3]. To determine the stability of the structures, Ab Initio molecular dynamic simulations, binding energy calculations, and phonon dispersion spectra analysis were carried out [4]. Additionally, electronic properties and charge density differences were also analyzed. Together, the structural and electronic analysis results show that there is good interaction between the heterostructure layers with favourable stability. This study suggests that the PtO₂/AlN heterostructure possesses great potential for use as an anode material.

Keywords: anode material, heterostructure, first-principles

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TOWARDS CONCURRENT ENHANCEMENT OF IONIC CONDUCTIVITY AND MECHANICAL PROPERTIES OF IONOGEL FOR FLEXIBLE SUPERCAPACITOR APPLICATIONS

Yi Xiang Neoh^a, Shawn Siu Lun Loo^a, Swee Tiam Tan^{a,*}, Yvonne Shuen Lann Choo^{a,*}

^a*Kelip-kelip! Center of Excellence for Light Enabling Technologies, School of Energy and Chemical Engineering, Xiamen University Malaysia, Sepang 43900 Selangor Darul Ehsan, Malaysia.*

**Corresponding authors: yvonne.choo@xmu.edu.my, sweetiam.tan@xmu.edu.my*

Abstract

Ionogels have garnered increasing attention as viable alternatives for electrolytes in supercapacitors. This is attributed to their high energy density, which is a result of their wide electrochemical stability window. However, there exists a trade-off between the ionic conductivity and mechanical strength, resulting in a loss of structural integrity and leakage, hindering the ionogel's subsequent applications. Herein, an ionogel with concurrent enhancement of ionic conductivity and mechanical performance was fabricated with the utilisation of irradiation time and in-situ polymerisation induced phase separation (PIPS). This approach allows for greater IL content to be incorporated without ion aggregation while enhancing tensile strength through increased cross-link density. By increasing the irradiation time from 5 minutes to 7 minutes, the tensile strength of the ionogel more than doubled. The ionic conductivity also increased by 20% to 5.51 mS/cm, which is the highest of PIPS ionogel fabricated for supercapacitor application. The practical applicability of the ionogel as a flexible supercapacitor was further demonstrated as the integrated device exhibited a high specific capacitance of 103 F/g at a current density of 0.5 A/g, along with an impressive energy density of 129 Wh/kg and a power density of 3.09 kW/kg. Moreover, the device has a high capacitance retention (93%) after 30000 cycles at 1 A/g. It is noteworthy that the device exhibited stable electrochemical performance, even when subjected to various bending conditions. This study presents irradiation time as a new approach for addressing the trade-off between mechanical strength and electrochemical performance in ionogels.

Keywords: Polymerization Induced Phase Separation, Flexible Supercapacitor, Ionogel, Irradiation Time, Ionic Conductivity

Ag-FUNCTIONALIZED h-BN NANO-HYBRID: SOLVOTHERMAL SYNTHESIS, MULTIFUNCTIONAL CHARACTERIZATIONS AND ANTI-MICROBIAL ACTIVITY ASSESSMENT

Md. Abdul Mannan^{*1}, Mirza Humaun Kabir Rube²

¹Department of Chemistry, Faculty of Science, Rajshahi University, Rajshahi-6205, Bangladesh,

² Department of Materials Science and Engineering, University of Rajshahi-6205, Bangladesh,

Corresponding author: Email: mannan.chem@ru.ac.bd

Abstract

In this study, the Ag diethyldithio carbamate complex was first created, and then, stable Ag doped h-BN nanohybrid powder was effectively synthesized under environmentally friendly solvothermal conditions at a low temperature of (100 °C) and a comparatively high temperature (220 °C). X-ray diffraction patterns revealed the pure crystal phase/structure and Ag NPs peak/phase of the Ag-doped h-BN sample that was synthesized at 100 °C. The Ag-doped h-BN coated with Ag NPs shows the recently discovered characteristic peaks for Ag NPs. Transmission electron microscopy is used to detect the SAED pattern, lattice structure, spacing, Ag coating, and Ag NPs, which have a size of about 7 nm. Ag-doped h-BN nano-hybrids' shape and particle sizes were examined using SEM analysis both before and after pathogen treatments. The presence of Ag, B, and N atoms was specifically verified by quantitative data and EDS spectral analyses. This evidence is supported by the XPS spectra which produced the corresponding peaks of Ag, B, and N elements. Furthermore, based on the EDS mappings of each element, the Ag-doped nano-hybrids generated at 100 °C have a nearly uniform distribution. The E2g vibration mode for the primary h-BN peak was shown by Raman spectra, indicating the better crystalline structure of both pure and Ag-doped h-BN nano-hybrids. Raman, Fourier transform infrared, and UV-Vis data were used to examine the local architecture and optical properties of the produced materials, respectively. All of the samples showed mass loss up to 800 °C, according to TGA data assessments. For energy storage, the moderate piezoelectric constant ($d_{33} = 136$ pC/N) and remnant ($P_r = 86$ pC/NCm²) were obtained at 30 °C. Moreover, other materials showed a strong diamagnetic nature because of their high band gap values and insulating character, whereas the Ag complex sample showed weak paramagnetic activity. Ag doped h-BN nano-hybrids powder exhibited moderate anti-microbial activity, especially in *E. coli* and *B. cereus* pathogens.

Keywords: Solvothermal synthesis, Ag-doped h-BN nano-hybrid, microstructure, EDS, antimicrobial activity

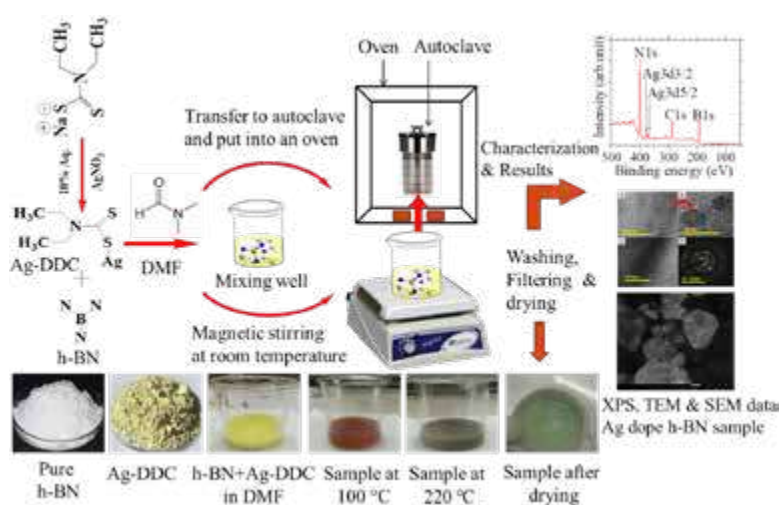


Figure 1. Synthesis scheme and primal characterizations of Ag-DDC complex and Ag doped h-BN by low temperature solvothermal method.

TAILORING POROUS ENGINEERING AND SURFACE MODIFICATIONS FOR ENHANCED LITHIUM-ION DIFFUSION

Jin-Cheol Kim^a, Woo-Jin Song^{a,b,c*}

^aDepartment of Chemical Engineering and Applied Chemistry, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^bDepartment of Material Science Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

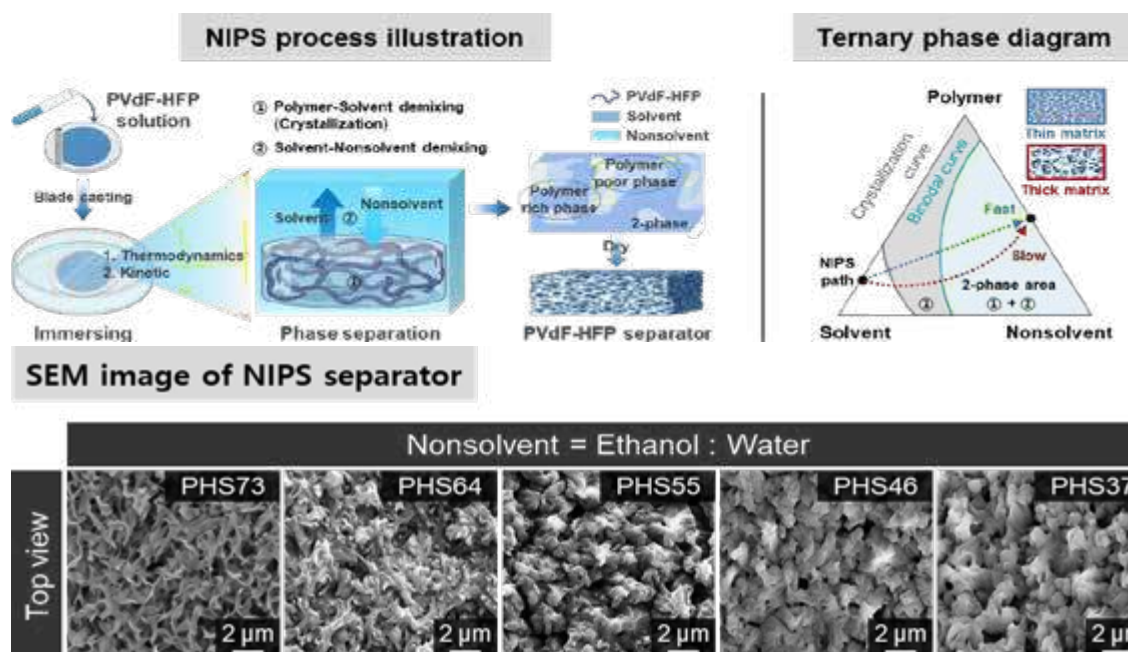
^cDepartment of Organic Materials Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

*Corresponding author: wjsong@cnu.ac.kr (W. -J. Song)

Abstract

The performance of lithium-ion batteries (LIBs) under rapid charging and elevated temperatures is significantly influenced by separator design.¹ In this work, we introduce a dual-engineering strategy that combines nonsolvent-induced phase separation (NIPS) with surface functionalization via polydopamine (PDA) spray coating. The modified separator, PHS73@PD, is fabricated from a PVdF-HFP matrix and exhibits a uniform porous architecture that enhances lithium-ion transport and diffusion uniformity. The PDA coating introduces polar functional groups that improve electrolyte wettability and facilitate ion mobility through electrostatic interactions.² This design effectively reduces polarization and internal resistance, leading to smoother lithium deposition and improved interface stability with lithium metal. Long-term cycling tests reveal that PHS73@PD maintains 82% capacity retention after 1000 cycles at 1C in full cells. This study demonstrates the potential of combining bulk porosity control and surface chemistry to develop advanced separators for fast and high-efficiency LIBs.

Keywords: PVdF-HFP, NIPS, polydopamine, separator, phase separation



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THREE-DIMENSIONAL POLYMER BINDER DESIGN WITH IMPROVED IONIC CONDUCTIVITY FOR ADVANCED LI-ION BATTERIES

Sanghyeon Woo^a, Woo-Jin Song^{a,b,c*}

^aDepartment of Chemical Engineering and Applied Chemistry, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^bDepartment of Material Science Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

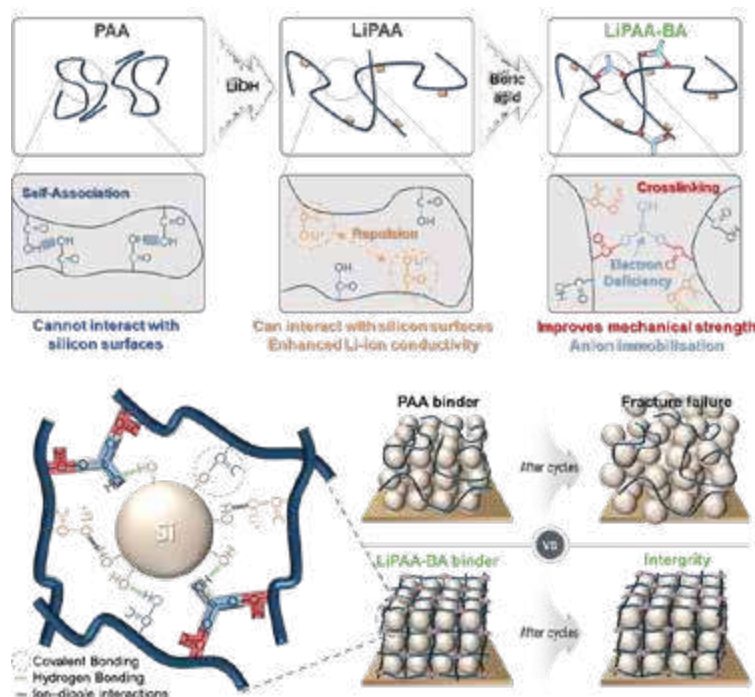
^cDepartment of Organic Materials Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

*Corresponding author: wjsong@cnu.ac.kr (W. -J. Song)

Abstract

Silicon (Si) anodes possess a high theoretical capacity ($\sim 4200 \text{ mAh g}^{-1}$), but their practical application is limited by the large volume change, unstable solid electrolyte interface (SEI) and low intrinsic conductivity.^{1,2} To address these issues, this study designed LiPAA-BA binders with a three-dimensional network structure by applying a pre-lithiation and cross-linking strategy to PAA. Compared to conventional linear PAA binders, LiPAA-BA indicates enhanced interfacial adhesion, mechanical strength, and Li-ion kinetics. The crosslinking agent adopted in this study has electron-deficient properties, which immobilise anions in the liquid electrolyte to facilitate the conduction of Li-ions and form a stable SEI layer. This approach differs from previous crosslinked binder studies that have primarily focused on improving mechanical strength, by expanding the role of the binder to modulating the solvation structure of Li-ions. As a result, the Si@LiPAA-BA electrode showed a capacity retention rate of about 100% after 300 cycles and increased the Li-ion diffusion coefficient by more than 1.6 times compared to the Si@PAA electrode with a previous linear PAA binder.

Keywords: Lithium-ion battery, Silicon anode, Polymeric binder, Cross-linked binder, Pre-lithiation



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CIRCULARLY POLARIZED LUMINESCENCE FROM ACHIRAL LANTHANIDE COMPLEXES VIA BIOMIMETIC REPLICATION OF SCARAB BEETLE ELYTRA

Nikita Madhukar^a, Takumi Kojima^a, Hitomi Ohmagari^a, Miki Hasegawa^{*a}

^aCollege of Science and Engineering, Aoyama Gakuin University, Japan

*Corresponding: hasemiki@chem.aoyama.ac.jp

Abstract

By imitating the complex structures that have evolved in nature, biomimetics presents a viable path towards the creation of functional materials.¹ By combining an achiral terbium(III) complex with a structurally duplicated template taken from the scarab beetle's elytra, we have created a unique photofunctional material that displays circularly polarized luminescence (CPL). The elytra's naturally occurring multilayered chitin-protein structure acts as a biomimetic model for the development of the CPL-active systems.² The elytra of the scarab beetle was used as a structural mold to integrate the synthesized terbium complex (TbLH)³, which is recognized for its f-f emission through the ligand to metal antenna effects, into solutions and cast onto replica films made from polyvinyl alcohol (PVA). The discussion will be based on spectroscopic analysis that confirms replication and functionalization. For instance, emission and excitation spectra showed strong green luminescence that corresponds to the $^5D_4 \rightarrow ^7F_j$ transitions of Tb^{3+} , and lifetime measurements showed multi-component decay, which indicates the heterogeneous environments in the solid state matrix. Most notably, CD measurement showed a Cotton effect around 290 nm, along with CPL signals at 491, 545, 586, and 622 nm, all demonstrating a g_{lum} value of approximately 0.01, which is sufficient to validate circular polarizability, as shown in Figure 1. Therefore, this study shows that the achiral TbLH complex imprinted with chiral environments to induce CPL, creating new opportunities for the development of optically active material from basic non-chiral building blocks. Potential uses for this newly developed photofunctional material include environmental sensing, information encryption and smart optical systems.

We acknowledge Prof. Masashi Hasegawa, Kitasato University, for the CPL measurements.

Keywords: Biomimetics, Elytra, Circularly polarized luminescence (CPL), Terbium, f-f emission

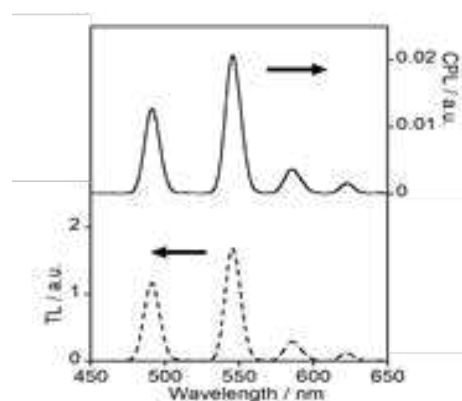


Figure 1. Circularly polarized luminescence (CPL) (solid line) and total luminescence (dotted line) spectra of TbC ($\lambda_{ex} = 315$ nm)

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CONTROLLED GROWTH OF POLYANILINE ON EPOXY FUNCTIONAL COTTON FABRIC AND INVESTIGATION OF ELECTROCHEMICAL PROPERTIES

Nergiz Cengiz^{a*}, Babajan Mahmutjanov^a, Tolga Karazehir^b

^a Tekirdağ Namık Kemal University, TÜRKİYE

^b Adana Alparslan Türkeş Science and Technology University, TÜRKİYE

*Corresponding author: ncengiz@nku.edu.tr

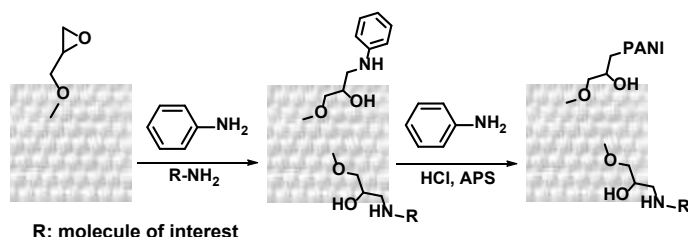
Abstract

Cotton is a natural resource that offers the purest form of cellulose and is one of the materials that cause the least harm to the ecosystem with its features such as sustainability and biodegradability. The rich hydroxyl groups of cotton-based natural materials facilitate surface modification to improve their properties for potential use in advanced polymeric materials. Polyaniline (PANI) is a conductive polymer that can be used in various applications with its impressive electrical conductivity, reversible redox properties, environmental durability, and anticorrosive properties. Although many studies have been conducted in the literature on uncontrolled coating of cotton fabrics with polyaniline to impart conductivity, uncontrolled coating brings disadvantages such as inhomogeneity of the coating, instability of electrical properties, and hydrophobicity.

In this study, we aimed to fabricate controlled PANI-coated cotton fabric. Cotton fabric was first treated with epichlorohydrin in basic medium to obtain epoxides. Then, aniline was attached to the epoxy-modified cotton fabric via epoxy-amine “click” chemistry, and PANI was grown by electropolymerization using ammonium persulfate (APS) in HCl solution following the addition of extra aniline to the fabric. A variety of conductive cotton fabrics were fabricated by varying parameters such as the ratio of aniline to APS, the concentration of HCl solution, and the temperature during the polymerization. The electrochemical characterization and electrical properties of cotton fabrics were investigated via cyclic voltammetry and electrochemical impedance spectroscopy. Moreover, multi-modifications with other amine containing molecules of interest will be discussed in this research. The results obtained from this study show that PANI-coated cotton fabrics with the presented method can be used as promising material in biosensor, electrocatalytic, and energy storage applications.

Keywords: PANI, conductive cotton fabric, chemical modification, click chemistry

Conductive and Functional Cotton Fabric Fabrication



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EPOXY-AMINE VITRIMERS TOWARDS ENHANCED RECYCLABILITY VIA DUAL-CHEMISTRY SYSTEMS

William E. Dyer^a, Niklas Lorenz^a, Baris Kumru^{a*}, Shermin S. Goh^b

^aAerospace Structures and Materials, TU Delft aerospace engineering, Kluyverweg 1, 2629 HS, Delft, Netherlands.

^bInstitute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR), 2 Fusionopolis Way, Innovis #08-03, Singapore 138634, Republic of Singapore.

*Corresponding author: b.kumru@tudelft.nl

Abstract

Epoxy-amine resins are an essential material in a variety of key industries including maritime, automotive, and aerospace. They are often used in the form of fibre reinforced polymer composites (FRPCs). Current resin formulations limit sustainable practices for material end of life in two ways. Firstly they do not allow for any reformability at end of life, leaving little room for designers to repurpose materials into new products. Secondly they provide no route for recyclability under mild conditions, with these harsh conditions (extreme pH, solvent, high temperature) leading to significant downgrades in material quality and a loss of value. The lack of recyclability leads to loss in value when dealing with carbon fibre composites (CFRPs) as the properties of the high value carbon fibres are degraded by harsh conditions.¹ Vitrimers present a potential alternative to this material wastage by enabling reformability, and many positive steps are being taken to translate knowledge from the vitrimer chemistry field to the nascent vitrimer engineering and processing field, enabling commercialization.² Disulfide chemistry has been utilized in much of this research due to its accessibility and compatibility with many epoxy systems. Whilst reformability is possible in pure disulfide vitrimers degradation of the matrix network for fibre recovery requires expensive, unstable reagents. Disulfide vitrimers are also prone to creep under high loads. Silyl ether bonds could address these issues as they are stable under normal conditions but have been shown to degrade under favorable aqueous acidic conditions. The following research explores the synthesis, formulation, and testing of epoxy-disulfide-silyl ether resin systems. These systems achieve medium-to-high T_g (+100°C), exhibit repeated network relaxation showcasing reformability, and network degradability via solvolysis at mild conditions showcasing recyclability.

Keywords: vitrimer, silyl ether, disulfide, sustainable composites, biobased

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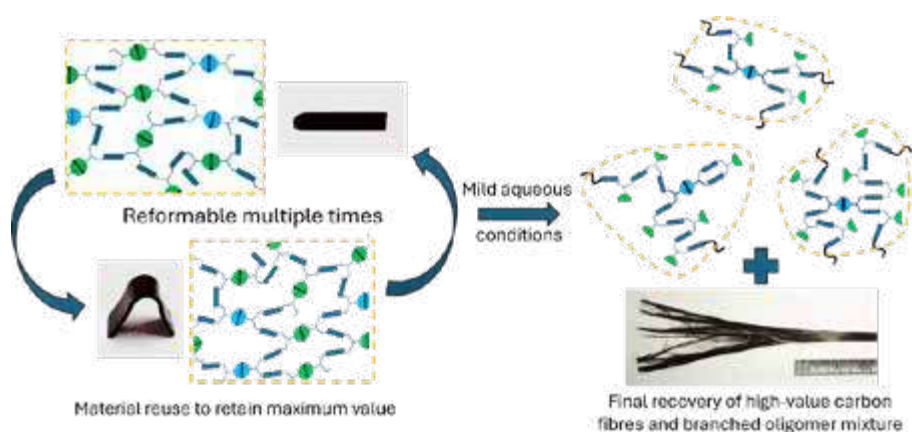


Image credit: Niklas Lorenz, DOI:10.1021/acsapm.4c03731 ; Wikipedia commons user: cjp24

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MECHANOCHEMICAL SURFACE ENGINEERING OF METAL OXIDES FOR ENHANCED PERFORMANCE IN HETEROGENEOUS CATALYSIS

Ana P.C. Ribeiro^{a,*}

^a Centro de Química Estrutural—Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1, 1049-001 Lisboa, Portugal

*Corresponding author: apribeiro@tecnico.ulisboa.pt

Abstract

Mechanochemistry has emerged as a sustainable and efficient method for the synthesis and modification of materials, offering solvent-free conditions and reduced energy requirements. In recent years, the mechanochemical treatment of metal oxides has shown significant potential in tailoring surface properties to improve their performance in heterogeneous catalysis.

This study aims to explore the mechanochemical activation of metal oxides to enhance their surface characteristics—such as surface area, defect sites, and dispersion—thereby improving their catalytic activity in heterogeneous catalytic reactions.

A series of metal oxides (including TiO₂, ZnO, and CeO₂) were subjected to high-energy ball milling under controlled conditions. The treated samples were characterized using X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) surface area analysis, transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). Catalytic performance was evaluated in model reactions such as CO oxidation and the selective oxidation of alcohols under flow conditions.

Mechanochemical processing significantly altered the physicochemical properties of the metal oxides. Increases in surface area (up to 2–3 times), generation of oxygen vacancies, and improved dispersion of active phases were observed. These modifications correlated with enhanced catalytic activity and selectivity. For instance, milled CeO₂ demonstrated a 40% increase in CO conversion at lower temperatures compared to the untreated material.

Mechanochemistry proves to be a versatile and green strategy for surface engineering of metal oxides, promoting the development of more efficient catalysts for heterogeneous catalysis. The method enables the fine-tuning of active sites without the need for high-temperature treatments or hazardous chemicals, underscoring its promise for scalable and sustainable catalytic material design.

Keywords: Mechanochemistry, metal oxides, heterogeneous catalysis, Green Chemistry

ANTI-FREEZING AND ANTI-DRYING CONDUCTIVE DOUBLE-NETWORK HYDROGEL WITH HIGH ELASTICITY

Nur Sara Batrishia Rosli^a, Nadia Adrus^{a,b*}, Muhammad Aqil Mohd Farizal^a, Tai Ji Zhang^a,
Muhammad Firdaus Mahmood^a, Jamarosliza Jamaluddin^{a,c}

^a*Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia*

^b*IJN-UTM Cardiovascular Engineering Centre, Institute of Human Centered Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia*

^c*Institute of Bioproduct Development, Universiti Teknologi Malaysia, 81310 Johor Bahru, Johor, Malaysia*

*Corresponding author: nadia@utm.my

Abstract

Hydrogels, soft and water-based materials with high biocompatibility and tunable mechanical properties, show great promise for biomedical uses. However, creating hydrogels that are both tough, conductive, and resistant to drying or freezing remains a challenge. This study introduces a double-network (DN) hydrogel, combining interpenetrating physical and chemical networks for superior toughness compared to single-network hydrogels. Calcium chloride (CaCl₂) is incorporated to enable conductivity, while immersion in a zwitterionic salt solution disrupts water hydrogen bonding, preventing ice formation. Monomers such as hydroxyethyl acrylamide (HEAAM) and acrylic acid (AA) are employed to optimize swelling and ionic properties. Therefore, the objective of this research is to produce an anti-dehydrating and anti-freezing DN conductive hydrogel with high swelling, conductivity, and mechanical properties. The DN conductive hydrogel was synthesized via a one-pot method using UV photopolymerization (365 nm, 15-minute curing), followed by 48-hour immersion in a zwitterionic salt solution and uniaxial stretching (2× ratio) to align its structure. The final hydrogel shows excellent properties: a high degree of swelling (3.8919), a gel fraction of 78.30%, and a freezing point below -50°C, confirming its anti-freezing capability. It can stretch up to 491.60% without breaking, has a tensile strength of 0.12 MPa, and conducts electricity efficiently (3.83×10^{-2} S/m), also proven by powering an LED bulb. Its high flexibility and durability make it ideal for wearable health sensors and medical devices that need to work in cold or dry environments. Its resistance to dehydration and extreme temperatures aligns with Sustainable Development Goal 3 (SDG3: Good Health and Well-being), supporting reliable health monitoring, prosthetics, or smart bandages in harsh conditions. With integrated conductivity, this hydrogel supports transformative solutions for continuous, accessible healthcare systems.

Keywords: Conductive hydrogel, Double-network hydrogel, Anti-freezing, Anti-dehydrating, Zwitterionic hydrogel

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RAPID UV LED PHOTOPOLYMERIZATION OF IONIC CONDUCTIVE AGAROSE-BASED HYDROGELS FOR ELECTRONIC SKIN APPLICATIONS

Muhammad Aqil Mohd Farizal^a, Nadia Adrus^{a,b*}, Nur Sara Batrishia Rosli^a,
Nur Syahirah Mokhtar^a, Jamarosliza Jamaluddin^{a,c}

^a*Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81310, Johor Bahru, Johor, Malaysia*

^b*IJN-UTM Cardiovascular Engineering Centre, Institute of Human Centered Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia*

^c*Institute of Bioproduct Development, Universiti Teknologi Malaysia, 81310 Johor Bahru, Johor, Malaysia*

*Corresponding author: nadia@utm.my

Abstract

Ultraviolet light emitting diode (UV LED) photopolymerization has become increasingly popular in producing polymers compared to the traditional UV mercury (UV Hg) photopolymerization, due to its environmentally friendly characteristics. One of the polymers that utilizes UV photopolymerization is hydrogel, a three-dimensional polymer network formed through physical and/or chemical crosslinking of hydrophilic monomers. Consequently, hydrogels, specifically ionic conductive hydrogels, are utilized in electronic skin applications, where exceptional attributes such as excellent flexibility, high conductivity, and responsiveness to external stimuli (e.g., light, pH, deformation, temperature, and humidity). However, the photoinitiators (PIs) for UV LED curing are limited since the absorption band of the PIs must overlap the narrow emission wavelength of UV LED. Furthermore, the commonly used PI for ionic conductive hydrogels, such as Irgacure 2959, was reported to have curing time ranges from 1 to 2 hours, which is relatively prolonged. In this study, a tough agarose/P(HEAAm-co-AA)/Ca²⁺ DN hydrogel was synthesized with the suitable concentration of PI at 2 wt.% of Chivacure 300 and 15 minutes of UV curing time via one-pot method and UV LED photopolymerization. The ionic conductive hydrogel exhibits an outstanding degree of conversion (99.91%), gel fraction (75.43%), degree of swelling (5.33), mechanical properties (~0.345 MPa tensile strength and ~525% elongation at break), anti-freezing (-0.84 °C), and conductivity (1.5 x 10⁻³ S/m). Therefore, the ionic conductive hydrogel of agarose/P(HEAAm-co-AA)/Ca²⁺ has the potential for electronic skin applications, synthesized via UV photopolymerization, which requires a lower curing time at a suitable PI concentration.

Keywords: UV LED, photopolymerization, photoinitiator, ionic conductive hydrogel, electronic skin

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SUSTAINABLE BIOBASED THERMOSETS FROM POLY (1,8-OCTANEDIOL-GLYCEROL-1,12-DODECANEDIOIC-ITACONIC ACID)

Najwa Wajihah Mohd Rusli^a, Nadia Adrus^{a,b,*}, Jamarosliza Jamaluddin^a Sani Amril Samsudin^a

^a*Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia*

^b*IJN-UTM Cardiovascular Engineering Centre, Institute of Human Centered Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia*

**Corresponding author: nadia@utm.my*

Abstract

Biobased polymeric materials offer a sustainable alternative to conventional thermosets. In this study, a fully biobased thermoset, poly (1,8-octanediol-glycerol-1,12-dodecanedioic acid-itaconate) (POGDIA), was synthesized via catalyst-free polyesterification using 1,8-octanediol, glycerol, 1,12-dodecanedioic acid and itaconic acid (IA) (0.5:0.5:1 molar ratio). The monomers employed are derived from renewable feedstocks: 1,8-octanediol and glycerol from plant oils and fermentation, 1,12-dodecanedioic acid from bio-based alkanes, and itaconic acid from microbial fermentation of carbohydrates, underscoring the green chemistry foundation of the synthesized thermoset. The prepolymer was crosslinked through thermal pre-curing (100 °C, 24 h) followed by UV irradiation with 2 wt% photo initiator (Chivacure 300). The resulting thermosets exhibited tunable properties depending on IA content and UV curing duration. The optimal formulation (20 phr IA) showed high conversion, increased gel fraction, and low swelling ratio. Fourier Transform Infrared Spectroscopy (FTIR) analysis confirmed the successful crosslinking through the disappearance of C=C stretching vibrations after curing, and SEM revealed uniform morphology. The material exhibited tensile strength of ~6.8 MPa and 110% elongation at break. Wettability improved with higher IA content, while DSC indicated a melting temperature of 54 °C with a shape memory transition starts around 35.7 °C. These properties, including tunable mechanical strength and shape memory characteristics, highlight POGDIA's potential for applications in soft actuators, coatings, and smart materials for biomedical devices.

Keywords: bio-based thermoset, shape memory polyester, shape memory polymer

HIGH-PERFORMANCE POLYMERIC ELECTRODE MATERIALS FOR ORGANIC BATTERIES

Febri Baskoro, Hui Qi Wong, Hung-Ju Yen*

^a Material Science and Engineering Research Group, Faculty of Mechanical and Aerospace Engineering,
Institut Teknologi Bandung, Bandung 40132, Indonesia.

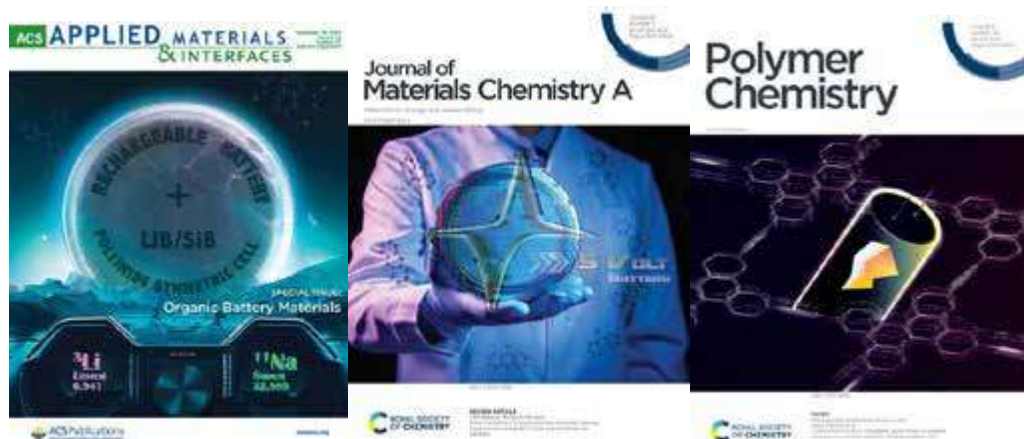
^b Institute of Chemistry, Academia Sinica, Taipei 11529, Taiwan

*Corresponding author: hjyen@gate.sinica.edu.tw

Abstract

Since lithium-ion batteries were first introduced, there have been numerous advances in cell design and cell chemistry. For example, the volumetric energy density has doubled, through a combination of improved active materials and better cell engineering. With the increasingly widespread use of lithium-ion batteries for new applications, the cells have been optimized for energy capacity (portable electronic devices, mobile phones and battery electric vehicles), or power (power tools, hybrid electric vehicles). For both the cell design and the active materials, there is a trade-off between power and energy capacity. This talk covers our recent works on high performance aromatic polymers as electrode materials for Li-ion batteries. Polymers with high thermal stability and thermo-oxidative stability complemented by excellent solvent resistance, good electrical and mechanical properties and chemical resistance make them as great candidate as electrode materials. Electrochemical performance tests reveal that these electrode materials delivered a reversible specific capacity and stability over thousand cycles. The long cycle lifetime and excellent battery performance further suggest that the reported polymers are promising electrode materials for next generation Li-ion batteries.

Keywords: polyamide, polyimide, lithium-ion battery, energy storage, organic electrode



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HYDROTHERMAL SYNTHESIS OF CERIUM OXIDE NANOPARTICLES AND THEIR PHOTODEGRADATION ASSESSMENT USING METHYLENE BLUE DYE

Muhammad Zamir Hossain^{a,*}, Shakira Billah Chaity^a, Lipi Akhter^a, Md. Mizanur Rahman^a, Bodrun Nahar^a, Md. Imran Islam^a, Nafees Ahmed^a, Gimyeong Seong^b

^aDepartment of Chemistry, Jagannath University, Dhaka 1100, Bangladesh

^bDepartment of Environmental and Energy Engineering, The University of Suwon, 17, Wauan-gil, Bongdam-eup, Hwaseong-si, Gyeonggi-do 18323, Republic of Korea.

*Corresponding author: Zamir@chem.jnu.ac.bd

Abstract

Currently, the discharge of methylene blue (MB) dye-containing wastewater is increasing as the textile printing and dyeing industry is developing. Wastewater-containing dyes are frequently treated using the photocatalytic method. Although several semiconductor metal oxide nanoparticles (NPs) are applied as a photocatalyst to degrade those dyes, however, very little effort is found using cerium oxide (CeO₂) NPs in this regard. In this article, CeO₂ NPs were synthesized via a hydrothermal method and tested their ability to photodegradation of MB dye in aqueous solution. First, hydrothermal experiments were investigated at 9 different temperatures and reaction times to set the optimum reaction condition for the formation of CeO₂ NPs. Ultraviolet-visible (UV-vis) spectroscopy, X-ray diffraction (XRD), transmission electron microscopy (TEM), high-resolution transmission electron microscopy (HRTEM), and Fourier transform infrared (FTIR) were used then to analyze the produced CeO₂ NPs. Analyzed data revealed that our efforts produced cubic CeO₂ NPs without the need for a surfactant or calcination step. The maximum degradation efficiency was calculated as 81.4% for 5 ppm MB dye solution which indicates that hydrothermally produced CeO₂ NPs are highly effective at photocatalyzing the breakdown of MB dye with the irradiation of UV light.

Keywords: Cerium oxide nanoparticles: hydrothermal synthesis: photocatalytic degradation: evaluation

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SYNTHESIS AND CHARACTERIZATION OF CHITOSAN FUNCTIONALIZED SALICYLALDEHYDE AND 2-ACETYLPHENOL-BASED THIOSEMICARBAZONES, AND THEIR ANTICANCER ACTIVITY

Hari Sharan Adhikari^{a,b,*}, Rameshwar Adhikari^{b,c,d}, Paras Nath Yadav^c

^a Pashchimanchal Campus, Institute of Engineering, Tribhuvan University, Pokhara, Nepal

^b Nepal Polymer Institute, Kathmandu, Nepal

^c Central Department of Chemistry, Tribhuvan University, Kathmandu, Nepal

^d Research Center for Applied Science and Technology, Tribhuvan University, Kathmandu, Nepal

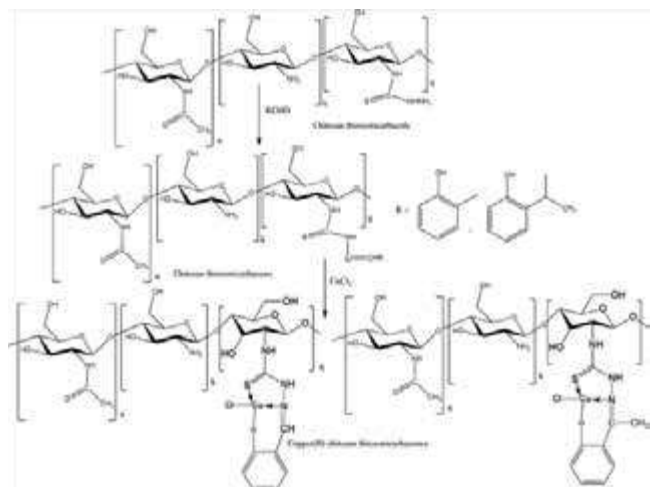
*Corresponding: adhikari687@gmail.com

Abstract

Functionalization of chitosan as salicylaldehyde and 2-acetylphenol-based chitosan thiosemicarbazone involving amino group at C2 position of pyranose ring and confirmation of the functionalization by comprehensive characterization by spectroscopic and analytical ways. Both the low molecular weight (M_w) chitosan oligosaccharide (CS) ($M_w < 3000$ Da, degree of deacetylation (DDA) = 87%) and the crab shell chitosan (CCS) ($M_w = 350$ k Da, DDA = 67%) functionalized thiosemicarbazones behaved as ONS tridentate ligand to form the square planar copper(II) complexes with a chloride ion as an additional ligand to satisfy the co-ordination sphere. All the derivatives were found thermally stable till the commencement of chitosan backbone disruption at 200 °C. The MTT assay profiles showed a conspicuous enhancement in the *in vitro* antitumorigenic and anticancer activity of native chitosan upon its functionalization as phenolic carbalddehyde chitosan thiosemicarbazones. Further, the assays more often revealed a further lowering of cell viability with chitosan oligosaccharide derivatives in comparison to high molecular weight chitosan derivatives, and a lower viability of the MCF-7 cancer cells than the tumorigenic MDCK cells. Both the low M_w chitosan with high DDA and high M_w chitosan with low DDA, the chitosan-functionalized salicylaldehyde based thiosemicarbazones, and their copper(II) chitosan thiosemicarbazone complexes were found to have minimal toxicity with $IC_{50} > 600 \mu\text{g mL}^{-1}$ against the mouse embryonic normal fibroblast NIH3T3 cells. These results were indicatives of more protonation and enhanced anticancer activity of chitosan oligosaccharide derivatives, and preferential cytotoxicity of chitosan biomaterials against the tumorigenic and cancer cells with more negatively charged cell surfaces. [1-2] Chelation of chitosan functionalized salicylaldehyde based thiosemicarbazones with copper(II) ions was also essentially important to lower the phenomenal involvement of copper(II) ions in tumor growth and proliferation. [3]

Keywords: 2-Acetyl phenol, Anticancer activity, Chitosan, Chitosan thiosemicarbazones, Copper (II) chitosan thiosemicarbazones, Functionalization, Salicylaldehyde

Graphical Image:



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BORON AND HYDROXYL FUNCTIONALIZED 3D CROSSLINKING BINDER FOR ENHANCED PERFORMANCE IN SILICON ANODES FOR LITHIUM-ION BATTERIES

Juwon Jeong^a, Shinyoung Lee^b, Jeonghun Kim^{c*}, Chang-Min Yoon^{d*}, Woo-Jin Song^{a,b,e*}

^a Department of Chemical Engineering and Applied Chemistry, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^b Department of Material Science Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^c Department of Chemical and Biomolecular Engineering, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea.

^d Department of Chemical and Biological Engineering, Hanbat National University, 125 Dongseo-daero, Yuseong-gu, Daejeon 34158, Republic of Korea.

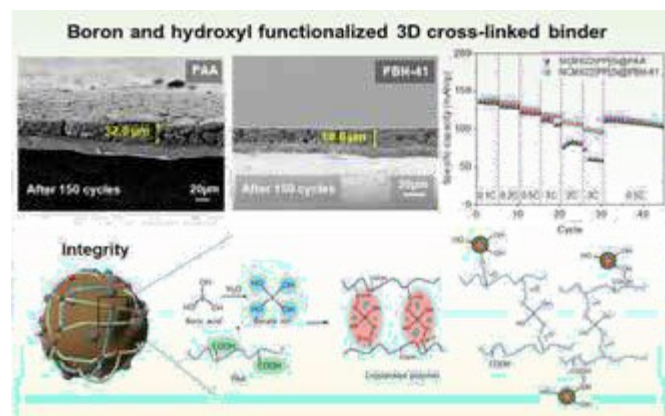
^e Department of Organic Materials Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

*Corresponding author: jhkim03@yonsei.ac.kr (J. Kim), cmyoon4321@hanbat.ac.kr (C.M. Yoon), wjsong@cnu.ac.kr (W. -J. Song)

Abstract

Silicon (Si) is one of the most promising anode materials for next-generation lithium-ion batteries, offering very high theoretical capacity (4200 mAh g^{-1}), far exceeding commercial graphite (372 mAh g^{-1}).¹ However, its practical use is limited by severe volume expansion during cycling and the formation of unstable solid electrolyte interphase (SEI), which leads to severe capacity degradation.² Binder design plays a critical role in controlling volume expansion and stabilizing the SEI layer during long-term cycling. This study aims to address the mechanical instability of Si anodes by designing high-performance binders that maintain structural integrity and enable long cycle life under high-capacity conditions. We developed a cross-linked polymer binder composed of poly(acrylic acid) (PAA) and boric acid (BA) to form a functional network containing electron-deficient boron and residual hydroxyl groups (PBH). Electrochemical evaluation showed that the PBH-based Si anode provided a high reversible capacity of 2275 mAh g^{-1} after 150 cycles, with an average Coulombic efficiency of 98.8% and a capacity retention rate of 88.85%. In addition, the whole cell paired with NCM622 cathode showed improved cycle stability for up to 100 cycles. These results demonstrate that the PBH binder significantly mitigates the volume change and improves the overall electrode integrity, providing a promising route towards stable and high-capacity Si-based Li-ion batteries.

Keywords: Lithium-ion batteries, Silicon anodes, Crosslinked binder, Boric acid



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Cu-Gr-TiO₂ TERNARY NANOCOMPOSITE FOR THE APPLICATION OF ANTICORROSION COATING: SYNTHESIS, CHARACTERIZATION AND ANTICORROSION PROPERTIES

Sook Ling Chng^a, Mui Yen Ho^{a*}, Ping Ping Chung^b, Peck Loo Kiew^c, Maxine Swee Li Yee^d

^a Centre of Advanced Materials, Faculty of Engineering and Technology, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Kelang, 53300 Kuala Lumpur, Malaysia.

^b Faculty of Engineering, Computing and Science, Swinburne University of Technology Sarawak Campus, Jalan Simpang Tiga, 93350 Kuching, Sarawak, Malaysia.

^c Department of Chemical and Environmental Engineering, Malaysia - Japan International Institute of Technology, Universiti Teknologi Malaysia, Jalan Sultan Yahya Petra, 54100 Kuala Lumpur, Malaysia.

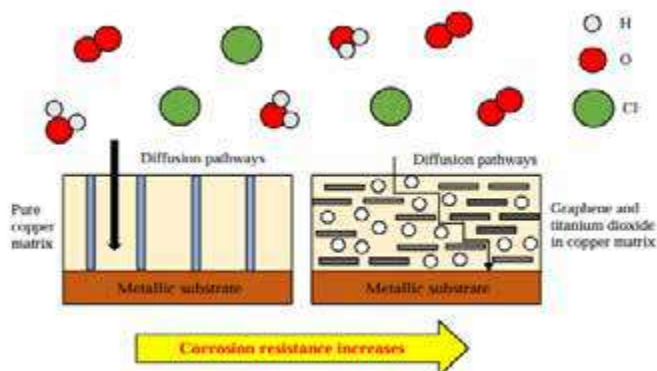
Department of Mechanical, Manufacturing and Materials Engineering, University of Nottingham Malaysia, Jalan Broga, 43500 Semenyih, Selangor, Malaysia.

*Correspondence: homy@tarc.edu.my

Abstract

In recent years, nanocomposite coatings have gained significant attention for anticorrosion applications due to their enhanced protective properties. This study reports the development of a novel ternary nanocomposite coating consisting of copper (Cu), graphene (Gr), and titanium dioxide (TiO₂) nanoparticles, synthesized via a simple one-step electrochemical deposition method. Graphene was produced through an environmentally friendly electrochemical exfoliation process in a mild sodium sulphate electrolyte. Characterization using scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), and thermogravimetric analysis (TGA) confirmed the successful formation of the Cu-Gr-TiO₂ nanocomposite. SEM revealed a denser and more compact surface morphology with fewer micropores upon the incorporation of graphene and TiO₂. EDX and XRD confirmed the presence of graphene and TiO₂ within the copper matrix. TGA indicated high thermal stability, attributed to the inherent thermal resistance of Cu and TiO₂. Peel-off tests showed improved adhesion strength due to the presence of TiO₂ nanoparticles. Corrosion resistance was evaluated in acidic (2% H₂SO₄) and saline (5% NaCl) environments using salt spray tests, electrochemical impedance spectroscopy (EIS), and potentiodynamic polarization. Among tested coatings—uncoated steel, pure Cu, Cu-Gr, and Cu-TiO₂—the Cu-Gr-TiO₂ coating exhibited the best corrosion resistance due to the synergistic barrier effect of graphene and TiO₂. The coating showed better performance in NaCl solution than in H₂SO₄. Corrosion protection efficiency reached 47.73% in salt spray tests. EIS revealed polarization resistance improvements of 82.29% in H₂SO₄ and 150.02% in NaCl. Potentiodynamic polarization indicated protection efficiencies of 45.45% and 64.10% in H₂SO₄ and NaCl, respectively, confirming the coating's excellent corrosion resistance.

Keywords: ternary nanocomposite; anticorrosion coating, graphene and TiO₂ within the copper matrix, electrochemical exfoliation



DEVELOPMENT OF A PCL-PDA-CU NANOFIBRE SCAFFOLD WITH CONTROLLED RELEASE OF COPPER IONS FOR ANTIBACTERIAL AND OSTEOGENIC SYNERGY

Tongbin Liu ^{1,2}, Akram Hassan ¹, Matheel Zohair Yousif Alrawas ¹, Zaihan Ariffin ^{1,□}

¹School of Dental Sciences, Universiti Sains Malaysia Health Campus, 16150, Kubang Kerian, Kelantan, Malaysia.

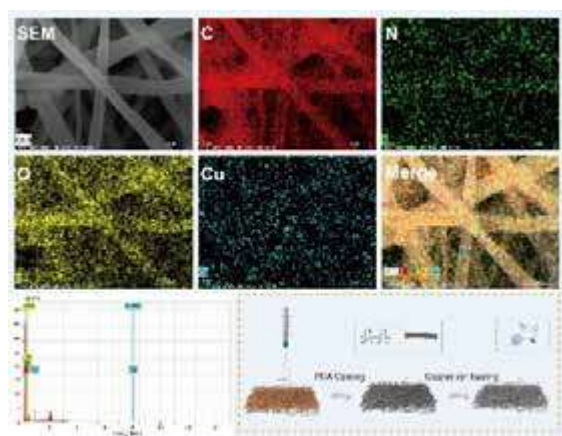
²School of Stomatology, Qilu Medical University, No. 1678 Renmin West Road, Zibo City, Shandong Province, China.

*Corresponding author: Zaihan Ariffin, zaihan@usm.my

Abstract

This study presents a nanofibrous material made from polycaprolactone (PCL) with a uniform polydopamine (PDA) coating on its surface. The catecholamine groups in PDA allow efficient chelation of copper ions, forming a stable complex and enhancing the biological functionality of the material¹. The PDA layer is evenly distributed over the PCL nanofibres and binds tightly to copper ions, resulting in a well-integrated composite structure. Structural and mechanical characterisation confirmed that the material has a stable three-dimensional architecture, favourable physicochemical properties and excellent mechanical strength, providing a strong basis for potential biomedical applications². Future work will explore the pH-responsive release behaviour of copper ions under different environmental conditions, aiming to mimic the mildly acidic microenvironments commonly associated with tissue injury or infection. In addition, the biological performance of the material will be systematically evaluated, in particular its application in bone tissue engineering, such as promoting bone regeneration and modulating the local microenvironment. Further optimisation of the copper ion release and reabsorption system will achieve a controlled balance between antibacterial activity and osteogenic potential, improving the overall therapeutic efficacy and biosafety of the material. This PCL-PDA-Cu composite shows great promise as a multifunctional and innovative scaffold for bone regeneration with controlled ion release capabilities³. It represents a compelling platform for future clinical translation and addresses key challenges in bone tissue engineering and regenerative medicine.

Keywords: Polycaprolactone; Polydopamine; Copper ions; pH-responsive; Antibacterial properties



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FROM SINGLE TO MULTI-ATOM CATALYSTS BY COVALENT ORGANIC FRAMEWORKS FOR HIGHLY EFFICIENT ELECTROCATALYTIC NITROGEN REDUCTION TO AMMONIA

Zhenjun Chang^{a*}, Fuxing Jia^a, Caikun Zhang^a, Ruiyong Chen^{b*}

^a*Jiangsu University of Science and Technology*

^b*University of Liverpool*

*Corresponding author: zjchang@just.edu.cn, ruiyong.chen@liverpool.ac.uk

Abstract

Under ambient conditions, electrocatalytic nitrogen reduction reaction is a feasible pathway with great development potential to replace the traditional Haber-Bosch process. It has the advantages of energy saving, low energy consumption and green environmental protection, which makes it one of the hotspots of current research^{1,2}. Designing and preparing high-performance catalysts to enhance ammonia yield and Faraday efficiency has become an important challenge. Single-atom catalysts show great potential in the field of electrocatalysis due to their advantages of high atom utilization and well-defined active sites. However, research on dual-atom or triple-atom catalysts for electrocatalytic nitrogen reduction is relatively scarce, particularly concerning the synthesis of covalent organic frameworks with well-defined active sites and their application in electrocatalytic nitrogen reduction. Moreover, the influence of individual atoms in dual-atom or triple-atom systems on the nitrogen reduction reaction remains unclear. Herein, we first prepared single-atom covalent organic framework catalysts by condensing cobalt tetraamino phthalocyanine and acenaphthenequinone, and then reintroduced second transition metal atom (Fe, Co, and Ni) to form dual-atom COF catalysts with well-defined structures using a simple impregnation method (Figure 1). Otherwise, using tetrakis(4-aminophenyl)porphyrin (TAPP) and acenaphthoquinone (ACQ) as precursors, a covalent organic framework (TAPP-ACQ) was synthesized via a solvothermal method. Subsequently, Fe, Co, and Ni transition metals were precisely anchored into the TAPP-ACQ framework through a solution impregnation approach, constructing dual-atom covalent organic frameworks (FeTAPP-FeACQ, CoTAPP-CoACQ, and NiTAPP-NiACQ) with well-defined active sites.

As a result, The design and preparation of high-performance catalysts exhibit superior catalytic performance in complex nitrogen reduction processes compared with traditional single-atom catalysts.

Keywords: nitrogen reduction reaction; covalent organic framework; single-atom; multi-atom catalysts

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UPCYCLING OIL PALM MESOCARP FIBERS: SUSTAINABLE TEMPO-OXIDIZED NANOCELLULOSE FOR ANTIMICROBIAL NANOCOMPOSITE HYDROGELS

Jeck Fei Ng^{a,*}, Jo Sze Lean^a, Siau Hui Mah^a, Soek Sin Teh^b,
 Harrison Lik Nang Lau^b, Yun Hin Taufiq-Yap^c

^aTaylor's University

^bMalaysian Palm Oil Board

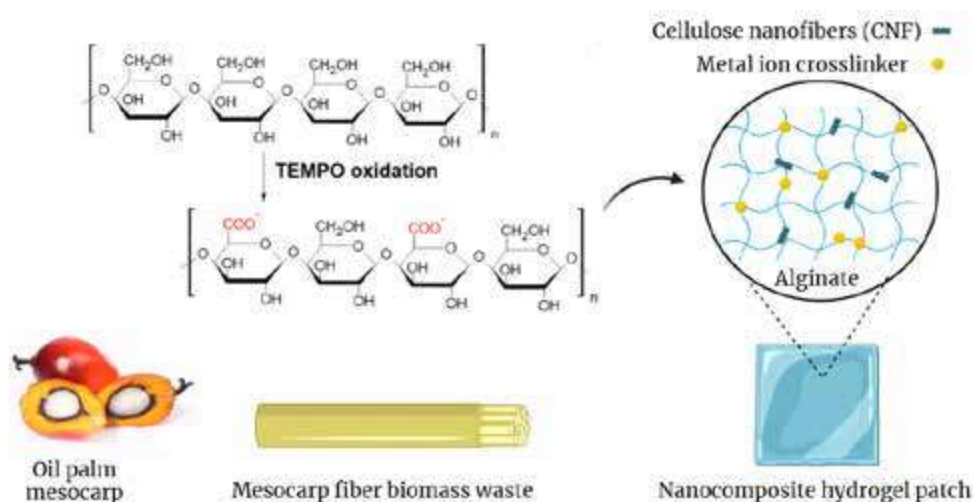
^cUniversity Putra Malaysia

*Corresponding author: jeckfei.ng@taylors.edu.my

Abstract

Oil Palm Mesocarp Fibers (OPMF) are under-utilised agriculture waste from the oil palm industry. This high lignocellulosic material can be used to produce high value commodities such as nanocellulose. Nanocellulose arises as a new class of futuristic nanomaterials to produce nanocomposite hydrogels due to their biocompatibility and potential surface functional groups modification for enhanced physicochemical properties. In the present work, nanocellulose originating from OPMF was successfully synthesised via TEMPO oxidation reaction. Under TEM imaging, the produced nanocellulose was elongated fibers-like in shape resulting in Cellulose Nanofibers (CNF) with 5-8 nm diameter. FTIR spectrum of the TEMPO-oxidised CNF showed identifiable carboxylate group on the surface indicating the successful modification of the surface functional groups. The degree of substitution of the carboxylate content was determined using conductometric titration and found to be 1.1 ± 0.12 mmol/g. This novel CNF exhibited excellent colloidal stability, as indicated by their zeta potential of -54.7 mV. Subsequently, mixtures of CNF and sodium alginate were crosslinked using six different metal cations. The resulting nanocomposite hydrogels showed significantly improved moisture uptake; moreover, the water stability of the hydrogels increases, indicating the improved physical strength of the hydrogels compared to pure crosslinked alginate hydrogels without CNF. Antimicrobial activities of the nanocomposite hydrogels were tested against *E. coli* and *S. aureus*. It was found that Ca^{2+} crosslinked nanocomposite hydrogels show no antimicrobial activity; while the microbial zone of inhibition of the nanocomposite hydrogels expands with different crosslinkers in the following order: $\text{Mn}^{2+} < \text{Cu}^{2+} < \text{Zn}^{2+} < \text{Ag}^+ < \text{Co}^{2+}$. Overall, the conversion of OPMF into high-value products minimises waste, supports a circular economy in agriculture, and enables the sustainable development of advanced applications like nanocomposite hydrogels for wound dressings.

Keywords: Oil palm mesocarp fibers, Nanocellulose, TEMPO-oxidation, Nanocomposite hydrogels, Antimicrobial



FABRICATION OF NANOSTRUCTURED ELECTRODE MATERIALS FOR SUSTAINABLE ENERGY APPLICATIONS

A. J. Saleh Ahammad*

Department of Chemistry, Jagannath University, Dhaka 1100, Bangladesh.

**Corresponding author: ajsahammad@chem.jnu.ac.bd*

Abstract

The development of efficient electrode materials is critical for advancing sustainable energy technologies, particularly in energy storage and conversion devices such as supercapacitors and water splitting systems. Porous carbon materials and nanostructured metal thin films have shown promising performance due to their high surface area and catalytic properties.

This study aims to fabricate and characterize porous carbon nanosheet and nanostructured rhodium (Rh) thin film electrodes for application in supercapacitors and oxygen evolution reaction (OER), respectively. Additionally, we investigate the influence of electrolyte composition on the electrocatalytic performance of Rh thin films.

Porous carbon nanosheets and Rh thin films were synthesized and characterized using FESEM, XPS, Raman spectroscopy, XRD, and N₂ adsorption-desorption analysis. The carbon nanosheets were tested as supercapacitor electrodes in a 1 M KCl neutral electrolyte. The Rh thin films were evaluated as electrodes for the oxygen evolution reaction (OER), examining the impact of different supporting electrolytes on their electrocatalytic activity through electroanalytical techniques and computational simulation methods.

The constructed supercapacitor showed an operating potential window of 1.1 V in 1 M KCl neutral electrolyte solution. At 2.25 A/g, the calculated specific energy was ~ 39.04 Wh/kg, along with a high specific power of ~ 1237.5 W/kg. The porous carbon material was able to retain specific energy of ~ 22.92 Wh/kg and specific power of ~ 41,250 W/kg at a high current density of 75 A/g. The Rh thin film electrode exhibited outstanding electrocatalytic activity for OER. Tafel slope (TS) analysis revealed that electron transfer kinetics was slower for the NaOH compared to the KOH electrolyte.

Porous carbon nanosheets and nanostructured Rh thin films are promising electrode materials for supercapacitors and water splitting, respectively. The carbon nanosheets exhibit excellent energy storage capabilities, while the Rh thin films demonstrate high OER activity, paving the way for advancements in sustainable energy technologies.

Keywords: porous carbon, rhodium, electrocatalyst, supercapacitor, oxygen evolution reaction.

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FUNCTIONAL BIOMATERIALS FOR WOUND HEALING: INNOVATIONS IN GELLAN GUM-BASED HYDROGEL SYSTEMS

Khairul Anuar Mat Amin*

Faculty of Science and Marine Environment, Universiti Malaysia Terengganu

21030 Kuala Nerus, Terengganu

**Corresponding author: kerol@umt.edu.my*

Abstract

The treatment of complex and chronic wounds remains a major clinical challenge, requiring materials that not only protect but also actively support tissue regeneration. In recent years, wound care research has shifted from passive barriers to dynamic, biofunctional systems that interact with biological processes to promote healing. In this work, we present the development of advanced wound dressing materials based on gellan gum, a naturally derived biopolymer known for its biocompatibility, hydrogel-forming capability, and structural versatility. To enhance its performance, we integrated several complementary components, each selected for specific biofunctional benefits. These include stingless bee honey from *Acacia* species ¹, which provides natural antioxidants and antimicrobial properties; collagen ², which mimics extracellular matrix structure and supports cell growth; titanium dioxide nanomaterials ³, which reinforce mechanical strength and confer antibacterial effects; and oil-filled microemulsions ⁴, which facilitate the controlled delivery of therapeutic agents. The resulting multifunctional hydrogels demonstrated improved wound healing potential in preclinical studies, with each modification guided by a clear design rationale aimed at optimizing mechanical integrity, biological compatibility, and therapeutic performance. This research highlights how the integration of naturally sourced ingredients with smart materials engineering can address critical challenges in wound management. In this presentation, I will share our interdisciplinary journey from material design to biological evaluation and discuss the broader implications for the future of bioengineered wound care solutions.

Keywords: gellan gum, honey, collagen, titanium dioxides, wound dressing

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FIELD-RESPONSIVE ALIGNMENT DYNAMICS IN CHIRAL NEMATIC LIQUID CRYSTALS: ESR INSIGHTS INTO HELICAL DIRECTOR DISTRIBUTIONS

Che Rozid Mamat and Rawaida Liyana Razalli

Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia.

**Corresponding author: cherozid@utm.my*

Abstract

Chiral nematic liquid crystals, known for their self-organized helical structures, exhibit unique field-responsive properties relevant to next-generation electro-optical systems. This study explores how magnetic fields influence director orientation in a cholesteric phase formed by doping an achiral liquid crystal (ZLI-4792) with cholesteryl propionate. The resulting helical arrangement is examined through Electron Spin Resonance (ESR) spectroscopy, which enables both qualitative visualization and quantitative measurement of director alignment. We derive an analytical form of the director distribution by solving the torque-balance equation and analyze how variations in dopant concentration and temperature affect the order parameter. Notably, higher chiral content induces a transition toward a more spatially isotropic (quasi-3D) distribution, where the helices become more randomized and lack a dominant alignment axis. Our ESR results align well with theoretical models and prior studies, providing deeper insight into how chiral dopants modulate director uniformity. These findings highlight the versatility of ESR spectroscopy as a tool to decode the alignment behaviour of complex liquid crystal systems and suggest new opportunities for tuning optical textures through molecular doping and external fields.

NANOFILTRATION MEMBRANE FOR DYE/SALT SEPARATION

Ying Zhang, Shencheng Pan, Xin Wang*

Key Laboratory for Soft Chemistry and Functional Materials of Ministry of Education, Nanjing University of Science and Technology, Nanjing 210094, China

*Corresponding author: wangx@njust.edu.cn

Abstract

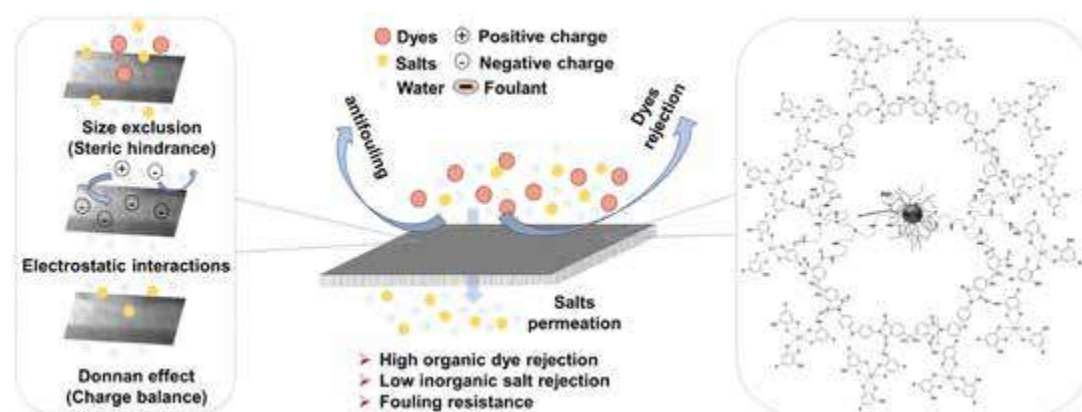
The textile industry, as a significant part of global manufacturing, generates large volumes of wastewater containing complex organic pollutants, heavy metal ions, and high concentrations of dyes during production processes. These contaminants pose severe threats to aquatic ecosystems and human health, exacerbating environmental pollution challenges. Meanwhile, increasing global water scarcity underscores the importance of wastewater reclamation and resource recovery. Loose nanofiltration is a cost-effective membrane separation technology that provides high separation efficiency. Its robust ability to intercept organic molecules and enhanced salt permeation position it as an exceptionally promising approach for treating textile wastewater. To this end, we have developed a loose nanofiltration membrane designed for efficient pollutant separation in water.

The substrate membrane is initially prepared using polyimides as the primary raw material, with nanodiamonds modified by polyethyleneimine integrated as an additive to enhance performance.¹ Subsequently, tannic acid and Fe^{3+} are introduced to form robust metal-polyphenol networks, culminating in the formation of a high-performance loose nanofiltration membrane. This type of nanofiltration membrane has the following advantages in structure and dye/salt separation applications:

1. Outstanding permeability of the loose nanofiltration membrane
2. Increased binding sites due to introduced amino groups
3. High pure water flux of $42.57 \text{ L m}^{-2} \text{ h}^{-1}$ in the loose nanofiltration membrane
4. High selectivity for organic dyes/inorganic salts separation (98.84)
5. Low rejection rate for inorganic salts (4.13%)
6. Demonstrated long-term stability during the separation process

In conclusion, the newly developed nanodiamond-modified membrane excels in dye/salt separation, showing great potential for broader wastewater treatment applications. Future plans include larger-scale trials to test scalability and address upscaling challenges.

Keywords: Wastewater treatment, nanofiltration membrane, dye/salt separation, nanodiamonds



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NANOARCHITECTONICS OF INDIUM SULFIDE/EXFOLIATED GRAPHITE/ MULTIWALLED-CARBON-NANOTUBES-BASED NANOCOMPOSITE IN BENZYL ALCOHOL AND ITS EFFECT ON AQUEOUS SYMMETRICAL SUPERCAPACITORS

Jian Hong Liew^a, Mui Yen Ho^b, Jyh Tsung Lee^c, Teck Hock Lim^{a*}

^a*Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Kuala Lumpur 53300, Malaysia.*

^b*Department of Manufacturing Technology, Faculty of Engineering and Technology, Tunku Abdul Rahman University of Management and Technology, Kuala Lumpur 53300, Malaysia.*

^c*Department of Chemistry, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan.*

**Corresponding author: limth@tarc.edu.my*

Abstract

Supercapacitors have garnered increasing attention as advanced energy storage devices, owing to their unique advantages and their potential to bridge the gap between conventional batteries and capacitors. A variety of materials, including indium sulfide and its composites with carbon-based materials, have been extensively studied as electrode materials for supercapacitors due to their ability to leverage both the pseudocapacitive (PC) and electric double-layer capacitance (EDLC) energy storage mechanisms. We have aimed at the synthesis and characterisation of indium sulfide and its composite, at the same time investigate their electrochemical properties and potential as supercapacitor's electrode. Herein, nanoscale indium sulfide was successfully deposited on a mixture of exfoliated graphite (EG) and multi-walled carbon nanotube (MWCNT) to produce a ternary nanocomposite in one step in polar benzyl alcohol. The 5-minute-to-completion synthesis was made possible via a rapid microwave-assisted thermolysis of indium acetate/thiosulfate mixture in the presence of a uniform dispersion of EG and MWCNT. The polar nature and high boiling point (205 °C) of benzyl alcohol helped to enhance product crystallinity, when compared to an analogue synthesis in which a non-polar solvent was used. The ternary nanocomposite was structurally characterized using a combination of PXRD, FESEM, HRTEM and EDX, with its electrochemical properties elucidated via cyclic voltammetry and galvanostatic charge/discharge. The ternary nanocomposite design was found to outperform its binary and singular counterparts with its Csp value registered to be 112 % higher than that quantified for the indium sulfide only counterpart. A respectable capacitance retention of 93% was observed for the ternary composite after 4000 cycles at a current density of 1.0 A/g, when paired with a mild aqueous sodium sulfite electrolyte. The performance of the nanoflower as an anode material for lithium-ion battery in a coin-cell assembly would also be discussed.

Keywords: Nanocomposite, Supercapacitor, Lithium-ion Batteries, Indium Sulfide nanoflower

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PROPOSING THE IMPRINTED PENA MODIFIED ELECTRODE FOR SPECIFIC DETERMINATION OF URINARY URIC ACID CONCENTRATION

Hsiao-Yu Cheng, Mei-Jywan Syu*

Department of Chemical Engineering, National Cheng Kung University

**Corresponding author: syumj@mail.ncku.edu.tw*

Abstract

Uric acid is the end product of purine metabolism. Abnormal uric acid level is related to gout and kidney diseases. Consequently, to measure uric acid concentration is essential and helpful to early diagnosis of these diseases.

In this work, we developed a molecularly imprinted polymer (MIP) sensor to determine the uric acid concentration in urine. 2-Ethyl-4-nitroaniline (ENA) was the functional monomer and a large proportion of crosslinker, EGDMA (ethylene glycol dimethacrylate), was added to achieve the interactions among the monomer, the uric acid template and the crosslinker. Thermo-polymerization was thus initiated in the presence of the initiator, AIBN (2,2-azobisisobutyronitrile). Via which, the uric acid imprinted poly(2-ethyl-4-nitroaniline) (PENA), in a film, was synthesized and fabricated onto the Au electrode. After which, the imbedded uric acid templates were washed out so that the specific binding cavities for uric acid molecules could be created. Thus, the cavities enable selective recognition and uptake of uric acid molecules. Differential pulse voltammetry (DPV) was utilized as the mode for electrochemical detection of uric acid. An imprinting factor of 10.1, as an index to evaluate the specificity of the MIP sensor towards uric acid with respect to the NIP (non-imprinted polymer) sensor, could be achieved. Additionally, the sensor thus prepared shows good linearity in the uric acid concentration range of 0~80 mg/dL. The cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were analyzed to understand the electrochemical characteristics of the MIP electrode and the others. Selectivity as well as storage stability of the MIP electrode were evaluated as well. The MIP sensor was further used to determine the uric acid concentrations in urine specimens, which were received from NCKU hospital (IRB approved: B-ER-110-510). Consequently, it could be concluded that the results show feasibility of the MIP sensor on clinical detection of uric acid concentration.

Keywords: uric acid, molecularly imprinted polymer, 2-ethyl-4-nitroaniline, differential pulse voltammetry, urine specimens

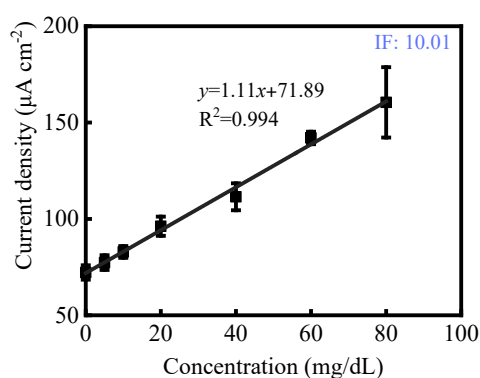


Fig. 1: Calibration curve of uric acid by the as-prepared MIP sensor.

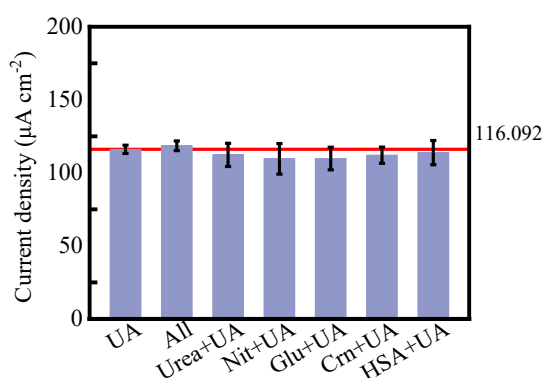


Fig. 2: Selectivity test of the MIP sensor.

ATOMISTIC INSIGHT INTO PHOTOVOLTAIC CELLS VIA 2D HETEROSTRUCTURE ENGINEERING

Opoku F^{a,*}, Govender PP^{a,*}

^aDepartment of Chemical Sciences, University of Johannesburg, South Africa

*Corresponding authors: ofrancis2010@gmail.com and pennyg@uj.ac.za

Abstract

A combination of different transition metal dichalcogenides (TMDs) leads to superior heterostructures where parameters such as charge transfer and strong interlayer interactions are significantly enhanced. We make use of the density functional theory method in this study to systematically explore the electronic structure, band alignment, interface charge transfers, mechanical and optical properties of $\text{MTe}_2/\text{GaTe}_2$ ($\text{M} = \text{Mo}$ and W) vdW heterostructures as a promising photovoltaic solar cell material. This work used gallium telluride and MTe_2 as acceptors and donors in high-quality photovoltaic cells. Calculated binding energies suggested that they were energetically favourable and easy enough to fabricate under suitable conditions. In addition, the heterostructures possess exceptional characteristics of enhanced visible light absorption edge ($\sim 104 \text{ nm}$), type-II band alignment and strong charge separation. The suitable band alignment led to a maximum power conversion efficiency (PCE) of 22.43 and 22.91%, respectively, which was quite promising for photovoltaic solar cells. The reason for the high PCE could be through the internal built-in electric field at the $\text{MTe}_2/\text{GaTe}_2$ interface, which induces efficient separation of charge carriers. This work offers theoretical support for the design and prediction of next-generation low-cost, highly efficient and promising materials for solar device applications.

Keywords: Power conversion efficiency, transition metal dichalcogenides, type-II band alignment, DFT, van der Waals heterostructures

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SYNTHESIS OF LOCUST BEAN GUM/TITANIUM DIOXIDE HYDROGEL NANOCOMPOSITES FOR METHYLENE BLUE REMOVAL

**Boitumelo Rejoice Motshabi^a, Kwena Desmond Modibane^a, Mpitloane Joseph Hato^a,
Orebotse Joseph Botlhoko^b, Mahmoud H. Abu Elella^c, Edwin Makhado^{a*}**

^a*Department of Chemistry, School of Physical and Mineral Sciences, University of Limpopo, Sovenga, 0727, Polokwane, South Africa*

^b*Centre for Nanostructures and Advanced Materials, DSI-CSIR Nanotechnology Innovation Centre, Council for Scientific and Industrial Research, Pretoria, 0001, South Africa*

^c*Chemistry Department, Faculty of Science, Cairo University, Giza, 12613, Egypt*

**Corresponding authors: edwin.makhado@ul.ac.za*

Abstract

The exponential pace of advancement has resulted in the emergence of water contamination as a significant environmental concern. In this study, hydrogel and hydrogel nanocomposite materials derived from grafted locust bean gum (LBG) were synthesised for the removal of methylene blue (MB) dye. Hydrogel and its nanocomposites were synthesised using the process of radical polymerization, both with and without the presence of TiO_2 . The produced samples' chemical composition and surface features were analysed using a variety of analytical tools, such as FTIR, SEM, XRD, and TEM. The Sips isotherm model was used to perform a batch adsorption experiment. The LBG-cl-p(AA-co-AAm) hydrogel has shown the ability to adsorb a maximum of 1406.7 mg/g of MB dye at a pH of 8. On the other hand, the LBG-cl-(AA-co-AAm)/ TiO_2 hydrogel nanocomposites exhibited a higher adsorption capacity, with a maximum of 1536.4 mg/g of MB dye. Based on thermodynamic data, it can be inferred that the removal of MB dye occurred as a result of spontaneous adsorption. Furthermore, the results of the regeneration experiment demonstrated that the hydrogel nanocomposites exhibited efficient recyclability for a total of six consecutive cycles. Hence, the hydrogel nanocomposites exhibit effective adsorption capabilities for the removal of MB dye from aqueous solutions.

Keywords: Locust Bean Gum, Wastewater Purification, Methylene blue, Hydrogel, Titanium Dioxide, Hydrogel Nanocomposite

UNVEILING THE POTENTIAL OF BMIMTFSI-FUNCTIONALIZED POLY(ACRYLIC ACID)-BASED IONOGEL POLYMER ELECTROLYTE FOR ELECTRICAL DOUBLE LAYER CAPACITOR (EDLC) APPLICATION

Kar Kien Ong^a, L.P. Teo^a, Chiam-Wen Liew^{a,*}

^a *Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Kelang, Setapak, 53300 Kuala Lumpur, Malaysia.*

**Corresponding author: liewchiamwen85@gmail.com; liewcw@tarc.edu.my*

Abstract

Ionogel polymer electrolytes (IGPEs) comprising poly(acrylic acid) (PAA) /lithium bis(trifluoromethanesulfonyl) imide (LiTFSI) /1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide (BmImTFSI) were prepared using the solution casting technique. PAA-based IGPE achieves a maximum ionic conductivity of (12.6 ± 0.01) mS/cm at ambient temperature upon addition of 35 wt.% of BmImTFSI and follows the Arrhenius theory which is based on temperature-activated model. In addition, infusion of BmImTFSI ionic liquid into the PAA backbone lowers the glass transition temperature to -7.77°C as confirmed by differential scanning calorimetry (DSC) study. Furthermore, the addition of ionic liquid in the PAA backbone improves the electrochemical potential and thermal stability of ionogel electrolyte, as proven in linear sweep voltammetry (LSV) and thermogravimetric analysis (TGA). Fourier Transform Infrared (FTIR) analysis proves the complexation between PAA, LiTFSI and BmImTFSI in the IGPE. An electrical double layer capacitor (EDLC) cell was fabricated using the highest conducting IGPEs and two identical carbon-based electrodes. The resulting EDLC cell exhibits superior electrochemical performances compared to the BmImTFSI-free gel polymer electrolyte. Upon the addition of BmImTFSI to the IGPEs, the EDLC shows an increase in specific capacitance from 10.25 F/g to 13.18 F/g, as illustrated in cyclic voltammetry studies. The results obtained are in good agreement with GCD findings. The fabricated EDLC achieves the power density of 59.96 W/kg and energy density of 0.99 Wh/kg.

Keywords: Polyacrylic acid; Ionogel; Ionic conductivity; EDLC; Specific capacitance

MIMICKING HUMAN THINKING FOR DISCOVERING NEW MATERIALS AND YIELDING NEW KNOWLEDGE IN AN EMERGING FIELD

Shuang-Yan Tian^a, Zhibo Ren^a, Yuting Zheng^a, Jingyi Wang^a, Xin-Yu Deng^a,
 Fanyang Mo^{a,b,c,*}, Ting Lei^{a,*}

^a*School of Materials Science and Engineering, Peking University, No.5 Yiheyuan Road, Haidian District, Beijing, 100871.*

^b*School of Advanced Materials, Peking University Shenzhen Graduate School, No.2199 Lishui Road, Nanshan District, Shenzhen, 518055.*

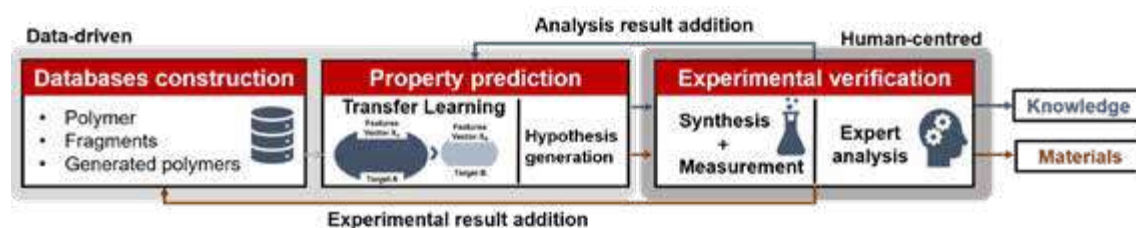
^c*Guangdong Provincial Key Laboratory of Nano-Micro Materials Research, Peking University Shenzhen Graduate School, No.2199 Lishui Road, Nanshan District, Shenzhen, 518055.*

*Corresponding author: fmo@pku.edu.cn, tinglei@pku.edu.cn.

Abstract

Artificial intelligence (AI)-driven materials development has emerged as a powerful alternative to traditional trial-and-error methods, which are inherently limited by human labor and cognitive capacity. Despite its promise, AI often struggles to uncover novel materials or generate actionable insights in emerging fields due to limited data availability. This challenge is particularly pronounced in electronic materials, where the intricate interplay of physical mechanisms and structure-property relationships impede progress. Here, we present a mimicking human thinking (MHT) materials development paradigm designed to facilitate both the screening of high-performance conjugated polymers and yielding materials knowledge in an emerging field. This workflow integrates: (1) transfer learning to address property prediction challenges for complex systems with limited data; (2) AI-driven hypothesis generation and feature selection based on materials science principles, providing essential insights into materials design; and (3) leveraging their expertise in synthesis, materials scientists select suitable molecules for synthesis and testing. Based on the test analysis results, they conduct knowledge embedding into the model and augment the training database. Using this approach, we successfully achieved an R^2 value exceeding 0.9 in predicting organic electrochemical transistor (OECT) carrier mobility, and V_{th} , screened high-performance n-type OECT polymers with values greater than 100 and V_{th} smaller than 0.1 V, and yielded new knowledge that significantly influence OECT polymers performance¹. We believe this paradigm can be applied to other emerging material systems characterized by limited data availability and complex physical mechanisms and accelerates the development of emerging material fields.

Keywords: polymer semiconductors; artificial intelligence; transfer learning; mimicking human thinking



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SYNTHESIS, CHARACTERIZATION, AND APPLICATION OF MAGNETIC S/Fe₃O₄ (SUFE0) NANOCOMPOSITE FOR HEAVY METAL CAPTURE AND ANTIMICROBIAL ACTIVITY

Yong Hong Shiow¹, Khatijah Yusoff², Vuanghao Lim³, Joon Ching Juan⁴, Rafidah binti Zainon³,
Chui Fung Loke¹, Teck Hock Lim¹

¹ Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Kuala Lumpur, 53300, Malaysia

² Department of Biochemistry and Microbiology, University Putra Malaysia, 43400 Serdang, Malaysia

³ Advanced Medical and Dental Institute, Universiti Sains Malaysia

⁴ Nanotechnology & Catalysis Research Centre, Institute of Advanced Studies, University of Malaya, Jalan Universiti, Kuala Lumpur 50603, Malaysia

*Corresponding author: shiowyh-wl21@student.tarc.edu.my

Abstract

This study presents the synthesis, structural characterization, and functional evaluation of a magnetic sulfur/iron oxide (“SUFE0”) nanocomposite as a magnetically recoverable agent for heavy metal capture and antimicrobial applications. SUFE0 was synthesized via chemical reduction of FeCl₃ using NaBH₄ to form Fe₃O₄ (IONP) nanoparticles in the presence of polyvinylpyrrolidone (PVP) as a non-toxic surfactant. Sulfur was heterogeneously deposited onto the IONPs via microwave-assisted melting at 180°C for 2 minutes, followed by rapid cooling to 55°C. Structural and morphological characterizations were conducted using PXRD, SEM, EDS and HRTEM, while magnetic properties were analysed by VSM. FTIR confirmed the presence of PVP in the nanocomposite. SUFE0 exhibited a uniformly spheroidal morphology with an average size of 710 nm. SUFE0 was capable of capturing 93% of Ag nanoparticle (Ag NPs) in water in 1.5 hr and the capturing process confirmed to follow a pseudo-second-order kinetic model. Additionally, SUFE0 exhibited antimicrobial activity against Gram-positive *Staphylococcus aureus* at a minimum inhibitory concentration of approximately 20,000 ppm. The findings highlight SUFE0’s potential as an environmentally friendly, magnetically separable material for heavy metal remediation and antimicrobial applications.

Keywords: green synthesis, iron oxide nanoparticles, heavy metal adsorption, magnetic nanocomposite, antimicrobial agent

Acknowledgement

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EFFECT OF METAL–ORGANIC FRAMEWORK ON HYDROGEN VOLUME FRACTION IN THE OXYGEN-RICH ANODE CATALYST LAYER OF PROTON EXCHANGE MEMBRANE WATER ELECTROLYZER

Keun-Hwan Oh^{a,*}, Inku Kang^a, Won-Jong Choi^a

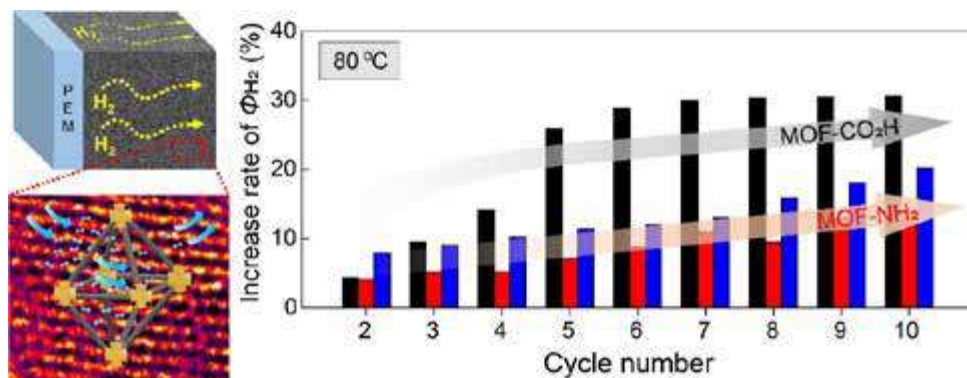
^aHydrogen Energy Research Center, Korea Research Institute of Chemical Technology, 141 Gajeong-ro, Yuseong-gu, Daejeon 34114, Republic of Korea.

*Corresponding author: khoh@kRICT.re.kr

Abstract

Hydrogen permeation through the membranes in proton exchange membrane water electrolyzers (PEMWEs) poses a significant safety risk, as the mixing of hydrogen with oxygen at the anode can lead to dangerous concentration levels and potential explosion hazards. This study investigates the modification of the anode catalyst layer (CL) within the membrane electrode assembly (MEA) to enhance the operational safety of PEMWEs by incorporating metal–organic frameworks (MOFs) with H₂-adsorbing capabilities. We evaluate the effects of MOFs with various functional groups on the H₂ concentration in O₂ stream and the electrochemical performance of the anode CL. The amine-functionalized MOF leads to the highest reduction in the H₂ concentration in O₂ stream. Additionally, the reversibility of the H₂ adsorption properties of the MOFs with temperature changes are verified. The amine-functionalized MOF leads to a H₂ volume fraction in O₂ of less than 1.2 mol% at the anode, which is well below the lower explosion limit of 4 mol% and thus, ensures PEMWE safety. In contrast, carboxyl and sulfonic acid-functionalized MOFs result in H₂ volume fractions in O₂ of 1.9 mol% and 2.2 mol%, respectively, at 50 mA cm⁻². These results provide crucial insights for developing safer anode CLs for PEMWEs.

Keywords: Hydrogen volume fraction, Metal–organic framework, Anode catalyst layer, Proton exchange membrane water electrolyzer



NOVEL TITIN-INSPIRED HIGH-PERFORMANCE POLYURETHANES WITH SELF-HEALING AND RECYCLABLE CAPACITIES BASED ON DUAL DYNAMIC NETWORK

Haopu Xie^a, Xiangdong Liu^a, Yuming Yang^{a*}

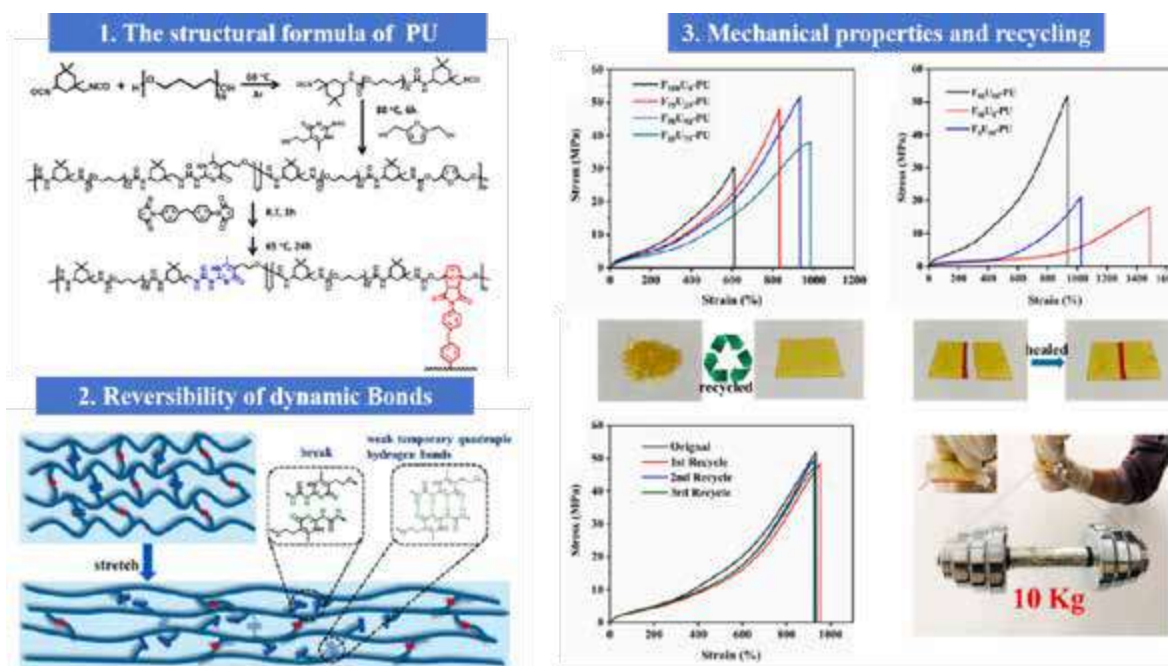
^aUniversity of Science and Technology of China

*Corresponding author: ymyang@ciac.ac.cn

Abstract

It is still a huge challenge that integrating excellent mechanical performance and high healing efficiency into self-healing materials at the same time, even if numerous dynamic bonds have been explored in preparing of self-healing materials in the last 20 years. Herein, we reported a novel titin-inspired strategy to prepare the polyurethanes via introducing dual dynamic network which contained the physical cross-linking of quadruple hydrogen bonds formed by 5-(2-hydroxyethyl)-6-methyl-2-aminouracil (UPy) dimers and the covalent cross-linking of Diels-Alder (D-A) bonds. Specially, relying on the synergistic effect of the dual dynamic network, the resulting polyurethane F₅₀U₅₀-PU exhibited admirable mechanical performance, such as a super-high strength of 51.9 MPa, a superb toughness of 166.7 MJ/m³ and a large elongation at break of 930%. Meanwhile, on account of the dynamic feature of quadruple hydrogen bonds and D-A bonds, the resulting polyurethane showed a high heat-induced healing efficiency of 91.2%. More importantly, the polyurethanes could be recycled by hot-pressing process to regain their initial mechanical properties and integrity. And it was also used as substrate to construct self-healing conductive device, which displayed splendid self-healing of electrical conductivity after damage. It can be envisioned that the polyurethanes with both superior mechanical performance and high healing efficiencies have great application prospect in multifarious fields.¹

Keywords: Titin-inspired, Dual dynamic network, Super-high strength, Self-healing, Recyclable



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FLUORINATED D–A–D TYPE π -CONJUGATED MOLECULAR CRYSTALS: 2D ELASTICITY AND ACTIVE OPTICAL WAVEGUIDE

Keigo Yano^a, Takumi Matsuo^a, Shotaro Hayashi^a

^a Kochi University of Technology.

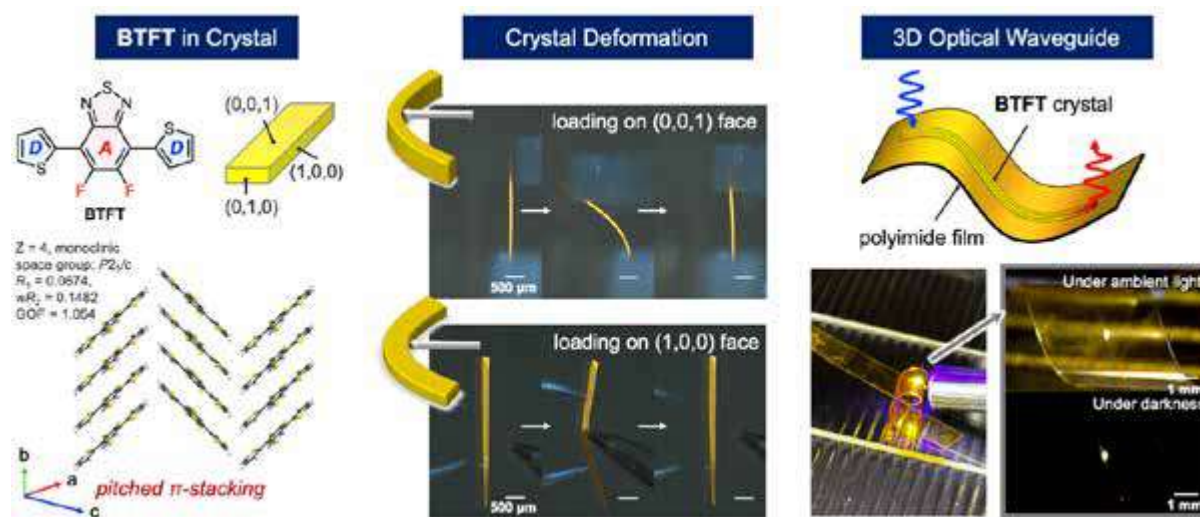
*Corresponding author: hayashi.shotaro@kochi-tech.ac.jp

Abstract

The diversity of organic molecular structures makes it possible to control their supramolecular self-assembly. Moreover, the self-assembly of π -conjugated molecules gives us a variety of functionalities for optoelectronic applications. Organic molecular crystals are important due to their density and anisotropic molecular alignments; however, such materials are less flexible in useful wearable materials. Robust and mechanically deformable organic molecular crystals, elastic crystals, are recently important in optoelectronic devices which differ from inorganic and polymeric solids.¹ However, it is well known that the understanding relationship between crystal structure and mechanical properties is difficult for elastic crystals. We have previously discovered that the pitched π - π stacking and 2D intermolecular interaction network structure in a crystal contributes to the elasticity of molecular crystals.^{2,3} In this study, we designed a Donor–Acceptor–Donor type fluorinated π -conjugated molecule, 4,7-bis(2-thienyl)-5,6-difluoro-2,1,3-benzothiadiazole (**BTFT**), resulting two-dimensional elasticity and yellow–PL characteristics in the molecular crystals.

Crystallization of **BTFT** was performed by a vapor diffusion (**BTFT** in chloroform with *n*-hexane) in a sample tube. The **BTFT** in crystal showed a highly planar molecular structure and pitched π -stack structure. This crystal shows elastic bending flexibility loading on both the (1,0,0) and (0,0,1) faces (2D elasticity). Since **BTFT** is a D–A–D molecule, the crystal offers yellow–PL. Furthermore, **BTFT** crystal was hybridized to a polyimide film which is excellent flexibility and optical transparency in the near-infrared region. The film is capable of loading the applied stress in multiple directions. We also present here a 3D optical waveguide based on the hybrid.

Keywords: Molecular crystal, Fluorinated π -conjugated structure, Elastic deformation, Optical waveguide, Doner-accepter-donor type



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MECHANICAL PROPERTIES OF ANTHRACENE-BASED HOST-GUEST COMPLEXES

Yuto Hino^a, Takumi Matsuo^a, Shotaro Hayashi^{a*}

^aKochi University of Technology

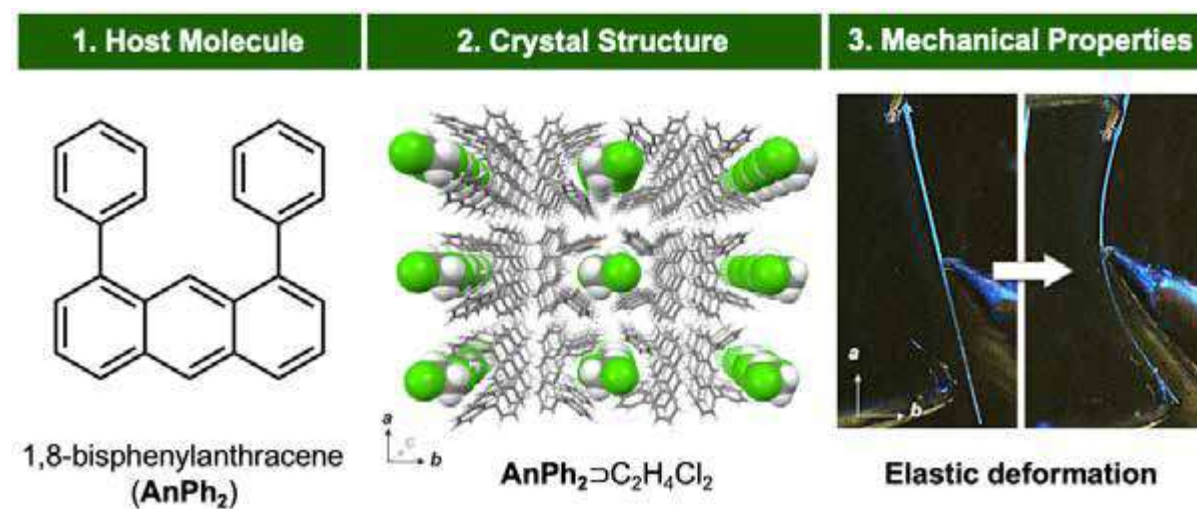
*Corresponding author: hayashi.shotaro@kochi-tech.ac.jp

Abstract

Host-guest molecular crystals are attractive in supramolecular chemistry. The crystallization, supramolecular self-assembly, of more than two molecules have opened the door of consorted functional materials. However flexible synthetic approaches are missing.

Organic molecular crystals are not flexible. This is because the intermolecular interaction in molecular crystals is thermodynamically stable and difficult to structural relaxation mechanism against external stress. Recently, studies on the mechanical deformation of organic molecular crystals have attracted much attention.¹ Designing flexibility is based on the columnar structure and the degree of freedom of intermolecular motion. Since the inclusion of guest molecules may ensure dynamic degrees of freedom in crystals,² it may be an important guideline for the creating the flexible and/or soft molecular crystals. Here, we have developed a host-guest complexation approach as a method to synthesize flexible and/or soft crystals. 1,8-Diphenylanthracene³ works as a host molecule, offering the voids formed between two phenyl groups for the captured guest molecules. The crystallization of 1,8-diphenylanthracene with a variety of guests yielded over twenty host-guest molecular crystals. Such crystals are similar 1,8-diphenylanthracene packing, but critically different mechanical properties were observed according to the guest molecules. In this presentation, we will discuss the details of these experiments, the crystal structure of the organic molecular cocrystals, and their mechanical properties.

Keywords: supermolecule, host-guest, single crystal X-ray diffraction, anthracene, phase transition



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HALF-FULL FILLED AEROGELS WITH A 348% INCREMENT IN ENERGY ABSORPTION AND A RETAINED HIGH ELECTROMAGNETIC SHIELDING PERFORMANCE

Ying Kong^a, Zhengqiang Lv^a, Changwei Li^a, Dongmei Hu^{a,*}

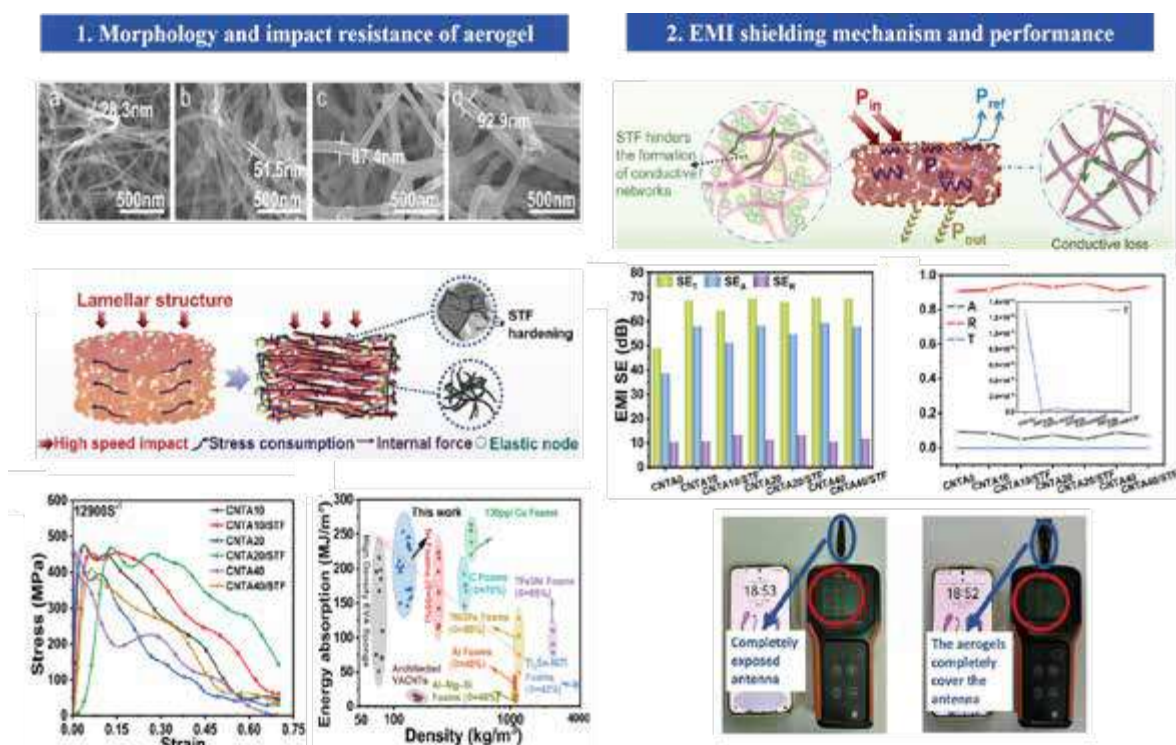
^aSuzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences

*Corresponding author: dmhu2010@sinano.ac.cn

Abstract

Aerogels, as kinetic energy absorbing materials, can find crucial applications for safeguarding in transportation, sports, buildings, construction, and aerospace. However, the highly porous structure makes it extremely fragile for endurance usage. In this study, a half-full filled structure has been proposed, and the concept has been demonstrated based on shear thickening fluid (STF) and chemically vapor deposited carbon nanotube aerogels (CNTAs), in which the outer part of CNTA is filled with STF while the inner core keeping unfilled. Chemical vapor deposition significantly enhances the elasticity and electromagnetic shielding performance of the native CNTA. The half-full filled aerogels (HFFA) show a 348% increase in energy absorption compared to the CNTA. At the same time, the density, electronic conductivity, and electromagnetic interference shielding effectiveness (EMI SE) of the HFFAs are 0.117 g cm^{-3} , 1213 S m^{-1} , and 69.52 dB (which is a neglectable reduction of 0.63% compared to native CNTA), respectively. The HFFA strategy provides an alternative route to fabricate robust aerogels with a remarkable increase of target properties while maintaining other properties, such as low density, high pore volume, and conductivity, with limited changes.¹

Keywords: Aerogels, Energy Absorption, Electromagnetic Shielding



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NANOFLOATING ARRAYS OF ORDERED ASSEMBLED GOLD NANOPARTICLES MODIFIED WITH POLYMER/AZOBENZENE DUAL-LIGANDS

Liangzhu Jiang^a, Renhua Deng^{a*}, Jintao Zhu^a

^aHuazhong University of Science and Technology, Wuhan 430074, China

*Email: rhdeng@hust.edu.cn

Abstract

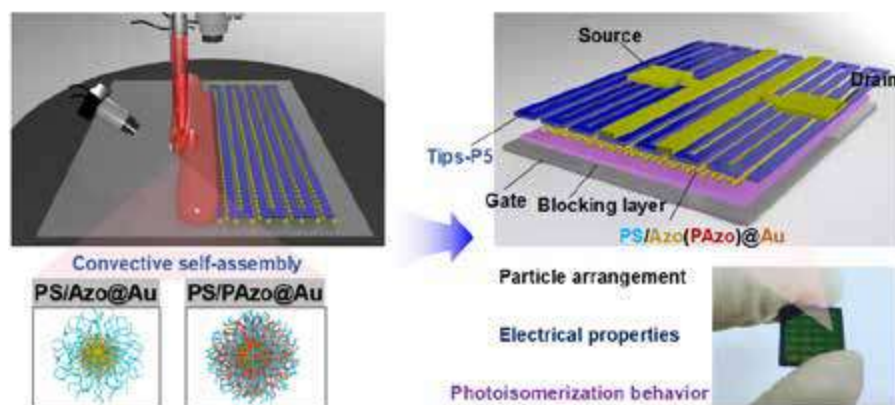
Nano-floating gate memory (NFGM) has emerged as one of the most promising next-generation memory devices. Our research focuses on NFGM based on organic ligand-modified gold nanoparticles, which exhibit excellent electrical properties and stable retention capabilities. To further enhance storage performance, we have functionalized gold nanoparticles using dual ligands composed of PS polymer and azobenzene molecules, leveraging the synergistic effects of these materials.

This discussion will focus on the following key points to explore methods for performance enhancement:

1. The assembly process of dual-ligand-modified nanoparticle arrays.
2. A comparative analysis between azobenzene small molecules and polymeric azobenzene in terms of surface composition, particle arrangement, and dielectric properties.
3. A comparison of device characteristics in devices based on gold nanoparticles with different ligands.

Finally, we have achieved exceptional storage performance in devices based on PS and polymeric azobenzene molecule-modified nanoparticles, demonstrating a memory window exceeding 50 V and stable retention capabilities. Additionally, we investigate the influence of photoisomerization behavior on device performance, revealing its potential for optical modulation in memory applications.

Keywords: nano-floating gate memory, organic ligand modification, gold nanoparticles, memory performance optimization



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FRET-ASSISTED OPTICAL WAVEGUIDE BASED ON FLEXIBLE MOLECULAR CRYSTALS

Koki Ikeda^a, Takumi Matsuo^{a,b}, Shotaro Hayashi^{a,b*}

^aSchool of Engineering Science, Kochi University of Technology

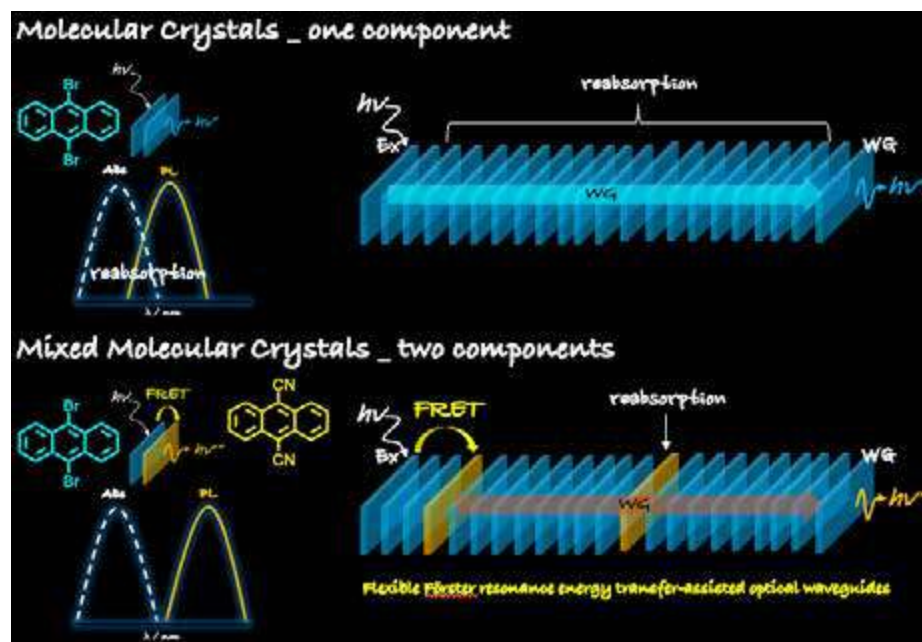
^bFOREST Center, Research Institute, Kochi University of Technology

*Corresponding author: hayashi.shotaro@kochi-tech.ac.jp

Abstract

Molecular crystal-based optical waveguides have recently become of interest as compact optical communication materials. Flexible molecular crystals are one of the candidates to realize wearable waveguides. However, both low emission efficiency and strong reabsorption in the crystal are problems regarding communication signal strength and high loss factor α (low photon transporting efficiency). The development and improvement of Förster resonance energy transfer (FRET)-assisted optical waveguides are a breakthrough approach for highly efficient optical waveguides. Herein we present elastic 9,10-dibromoanthracene-based molecular crystals doped with electron-accepting 9,10-substituted anthracene, anthracene-based elastic mixed molecular crystals.

Anthracene acceptors (9,10-diformylanthracene or 9,10-dicyanoanthracene) were selected as the dopant for solution-growth (crystallization) of 9,10-dibromoanthracene. ¹H NMR measurements of the obtained mixed crystals resulted in the acceptor doping to be 1%-5%. Elastic and fluorescent properties were maintained even when doped with such a few percent of the acceptor. The α value of 1%-doped crystals is much lower than that of the crystal consisting of only 9,10-dibromoanthracene crystal due to the reduced reabsorption in the FRET system. We have successfully demonstrated a practical approach for developing highly efficient and flexible optical waveguides.



Keywords: Optical Waveguides, Flexible Crystals, Anthracene

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EFFECT OF THE COOLING TEMPERATURE ON MECHANICAL PROPERTIES OF PPS COMPOSITES WITH HIGH LOADING OF GF FOR FILM CAPACITOR HOUSING

Seo-Hwa Hong¹, Pyoung Chan Lee^{1*}, Beom-Gon Cho^{2*}

¹Chemical Materials R&D Department, Chassis & Materials Research Laboratory, Korea Automotive Technology Institute, 303 Pungse-ro, Cheonan-si 31214, Chungnam, Republic of Korea

²Department of Polymer Science and Engineering, Kumoh National Institute of Technology, 61 Daehak-ro, Gumi, Gyeongbuk 39177, Republic of Korea

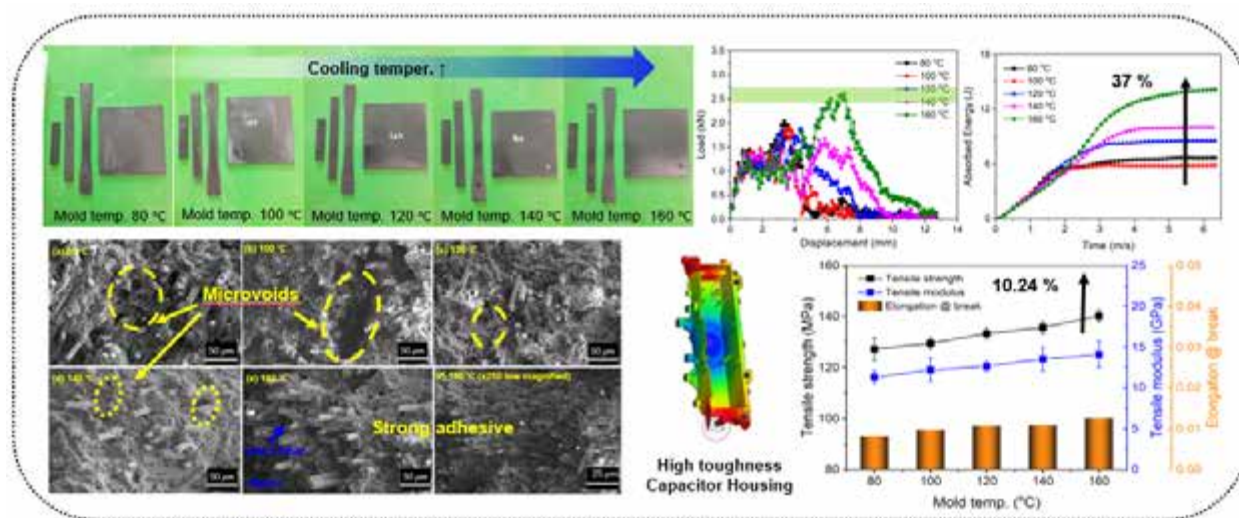
*Corresponding author: shhong1@katech.re.kr

Abstract

Capacitor materials must exhibit high thermal stability and low shrinkage to maintain long-term performance. Poly (phenylene sulfide) (PPS) is a high-performance engineering plastic with excellent rigidity, chemical resistance, and electrical insulation properties. Meanwhile, PPS composites with high glass fiber (GF) content enhances the mechanical properties of PPS, expanding its application potential.

However, the crystallinity and mechanical properties of PPS/GF composites have been found to vary depending on the cooling temperature. In this study, PPS/GF composites were fabricated via injection molding under different cooling conditions to investigate their mechanical and crystalline properties. The results indicate that higher mold temperatures allow sufficient crystallization time, leading to increased crystallinity. This enhanced crystallinity contributes to improved mechanical performance, as demonstrated by higher tensile, flexural, and impact strength. Fracture surface analysis of impact-tested specimens provided insights into GF orientation and microspore morphology. These findings contribute to optimizing the processing conditions of PPS/GF composites, making them more suitable for high-performance capacitor housing applications.

Keywords: Poly (phenylene sulfide), Glass fiber, Injection molding, Cooling temperature, Composite



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SYNTHESIS, PHOTOPHYSICAL AND ELECTROCHEMICAL PROPERTIES OF DI(1-BENZOTHIENO) [3,2-*B*:2',3'-*D*]PYRROLE DERIVATIVES WITH D- π -D TYPE STRUCTURAL CONFIGURATION

Chih-Jung Hsu, Yung-Sheng Yen*

Department of Chemistry, Chung Yuan Christian University.

*Corresponding author: ysyen@cycu.edu.tw

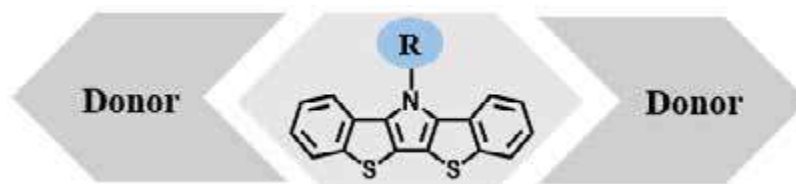
Abstract

Perovskite solar cells (PSCs) have garnered significant attention in photovoltaic technology due to their rapid development and high efficiency potential. A key component of PSCs is the hole transport material (HTM), which facilitates the extraction and transport of holes from the perovskite absorber to the electrode. Among the various HTMs, organic small molecule HTMs have emerged as promising candidates due to their tunable properties, solution processability, and potential for high performance.

In this study, we have developed three D- π -D type hole transport materials (DBTP-1, DBTP-2, and DBTP-3) for application in perovskite solar cells. These materials are based on di(1-benzothieno)[3,2-*b*:2',3'-*d*]pyrrole (DBTP),^{1,2} a fused heterocyclic π -conjugated system known for its excellent charge transport properties, high thermal stability, and strong electron-donating ability. The DBTP core structure enhances molecular planarity and π - π stacking interactions, which are beneficial for efficient hole transport in PSCs.

A series of di(1-benzothieno)[3,2-*b*:2',3'-*d*]pyrrole-based derivatives were successfully designed and synthesized for PSC application. The photophysical properties, redox behavior, and thermal properties of synthesized materials were investigated. Our findings suggest that this series of DBTP derivatives holds significant potential for application in perovskite solar cells.

Keywords: perovskite solar cells, hole transport materials



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APPLICATION OF POLYMETHYLETHOXYSILOXANE-POLYETHYLENE GLYCOL AND SILICA SOL IN ETHYLCELLULOSE IN CEMENT SYSTEMS AS MODIFIERS

N.Ye.Bekturganova^{a,b*}, I.V. Kolesnikova^b, N.O. Samenova^c, A.S. Suvorov^d

^{a,b*} Kazakh Automobile and Road Institute named L.Goncharov,

^b International Educational Corporation

^c Institute of Metallurgy and Ore Beneficiation

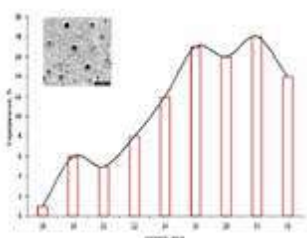
^d "SAPA INTERSYSTEM"LL,

*Corresponding author: bektur_n@mail.ru

Abstract

Obtaining widely demanded high-strength concrete from local raw materials, including modifiers - one of the current issues of science in Kazakhstan. The aim of the studies, the results of which are presented in the article, is to study the influence on the physical-mechanical properties of cement systems of synthetic hydrophobic additives: product based on polymethylethoxysiloxane - polyethylene glycol (PMEOS -PEG) and a product representing silicosol in ethyl cellulose (Silicasol). PMEOS -PEG has been found to increase the mobility of the solvent mixture, and also slightly increases the latency; Silicasol does not affect mobility and has a significant retarding effect. The introduction of the hydrophobizer PMEOS -PEG increases the strength of the mixtures by 50% when using Portland cement grade CEM II/A-S 42.5 N, and by 20% in mixtures with unmodified Portland cement CEM I 42.5 N. The addition of Silicasol does not change the strength characteristics of cement-sand mixtures, with a tendency for a slight decrease when using CEM I 42.5 N. The water resistance of concrete samples with the use of PMEOS-PEG and Silicasol additives at a dosage of 0.7% increased from W6 (without additives) to W12 and W8, respectively.

Keywords: polymethylethoxysiloxane, hydrophobic organic additives, concrete mixture, water resistance of concrete patterns



DYE INCLUSION AND AGGREGATION CONTROL USING STIMULI-RESPONSIVE COPOLYMER WITH CYCLODEXTRIN HOSTS

Shintaro Kawano^{a*}, Jenni Lie^b, Masahiro Muraoka^c, Motohiro Shizuma^a

^aOsaka Research Institute of Industrial Science and Technology

^bWidya Mandala Surabaya Catholic University

^cOsaka Institute of Technology

*Corresponding author: skawano@orist.jp

Abstract

Cyclodextrin (CD) is a cyclic oligosaccharide with a hydrophobic cavity and a hydrophilic exterior. It is a well-known host molecule and is capable of selectively recognizing guest molecules, which fit into its inner cavity. In particular, research into such drug loading and delivery based on host–guest interactions using β -cyclodextrin (β -CD) hosts in amphiphilic polymers has intensified. In our study, the stimuli-responsive copolymer comprising β -CD hosts has been utilized to aggregation and flocculation control by altering the hydrophilic/lipophilic balance (HLB) through hydrophobic interaction after inclusion of lipophilic dye molecules into the host cavity. The strategy can be potential application for removal of dye contaminants from wastewater environment.

Poly (*N*-isopropylacrylamide-co-acrylic acid) substituted with aminoethyl acrylamide- β -CD pendant groups (poly (NIPAM-AA- β -CD)), was synthesized by free radical copolymerization at appropriate molar ratio (**Figure 1A**), where the copolymer has thermo- and pH-responsive segments with molecular recognition sites. The ability of poly (NIPAM-AA- β -CD) to dissolve a lipophilic dye, i.e., Nile red (NR), changed in terms of the solubilization amount of NR according to the pH condition. The lower critical solution temperature (LCST) of the NR-incorporated poly (NIPAM-AA- β -CD) solution, which indicates its phase transition behavior, decreased at pH 4.0 owing to ionic complexation and an increase in hydrophobicity resulting from the inclusion of NR (**Figure 1B**).¹

Herein, we will present the results, indicating that the polymeric amphiphilicity can be modulated by host-guest interaction in the presence of a lipophilic dye to induce assembly and phase transition under precise pH control. The modulation of responsiveness of copolymers has great potential for use as water remediation adsorbents to induce aggregation and flocculation behavior even in the water-soluble material.

Keywords: stimuli-responsive polymer, cyclodextrin, host-guest interaction, organic dye

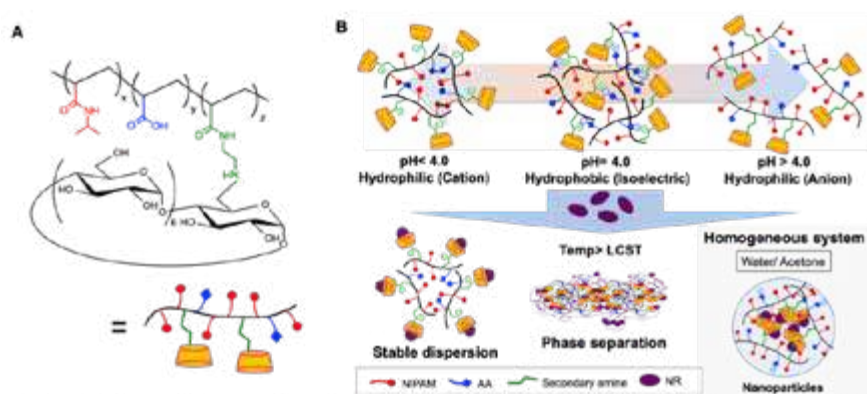


Figure 1 Chemical structure of copolymer (A) and stimuli-responsive behavior of the copolymer (B).

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SYNTHESIS OF π -CONJUGATED MOLECULAR CO-CRYSTAL TOWARD ANISOTROPIC PHOTON TRANSPORT

Mahiro Nakabayashi^a, Matsuo Takumi^{a, b}, Shotaro Hayashi^{a, b*}

^a School of Engineering Science, Kochi University of Technology

^b Research Institute, Kochi University of Technology

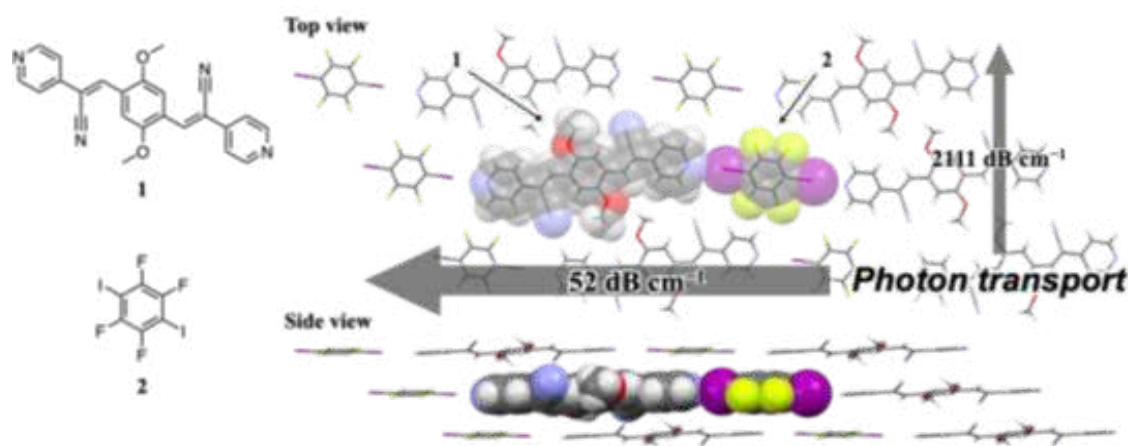
*Corresponding author: hayashi.shotaro@kochi-tech.ac.jp

Abstract

The high molecular density of organic crystals results in photon confinement and transport. Based on these features, molecular crystals have potential applications in optical logic circuits such as optical waveguides, resonators, and lasers.^{1, 2} Recently, photonics focused on the molecular anisotropy of crystals has attracted much attention. For example, anisotropic waveguides with different photon transport efficiency depending on crystal orientation have been reported.³ This phenomenon is based on the transition dipole moment of the molecule. Crystals with highly one-dimensional molecular orientation provide enhanced photon transport in specific directions. Therefore, crystal engineering based on precisely controlled intermolecular interactions can be expected to develop better anisotropic waveguides.

Here, we have synthesized the co-crystal with one-dimensional arrangements of luminescent molecules using intermolecular halogen bonding. The co-crystal was synthesized by a solution growth of pyridyl-terminated luminescent π -conjugated molecule **1** with 1,4-diiodo-2,3,5,6-tetrafluorobenzene **2**. Single-crystal X-ray structure analysis of the co-crystal shows that the strongly directional interaction between the lone pair of the pyridyl and the σ -hole of the iodine group is effective for one-dimensional alternating arrangement. Thus, the attenuation coefficient in the optical waveguide was measured on the short-axis and long-axis direction of the co-crystal. Interestingly, the attenuation coefficient ratios differed by a factor of about 40, indicating that the co-crystal has strong anisotropic photon transport capability.⁴ This co-crystal is superior compared to previous anisotropic wave guides.

Keywords: π -conjugated molecule, molecular co-crystal, halogen bonding, anisotropic optical waveguide, photonic logic gate



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CYANATE RESIN COMPOSITE MATERIAL

Yijia Zhou^{a*}, Chunhua Zhang^a

^aHarbin Institute of Technology,

*Corresponding author: zhouyijia1998@163.com

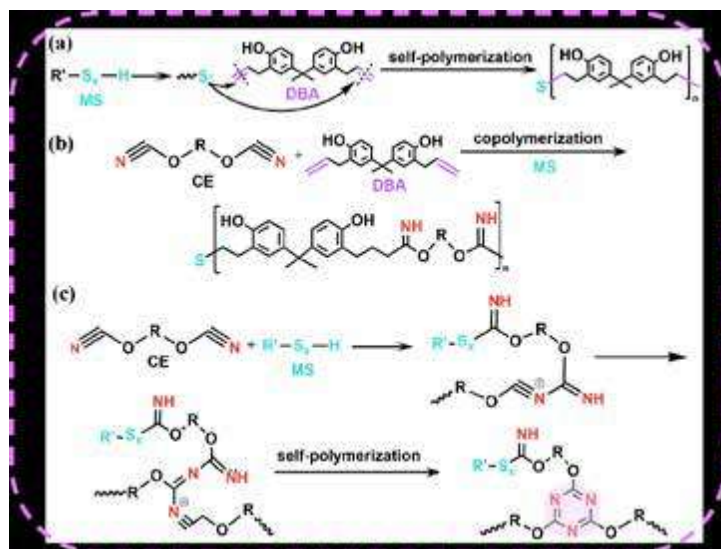
Abstract

Cyanate ester (CE) resin has excellent advantages in heat resistance, mechanical properties, and interfacial adhesion, and composite materials prepared with CF have broad application prospects in aerospace materials. However, addressing the inherent brittleness and high curing and molding temperatures of CE remains a top priority. The resin system prepared in this study has the following highlights.

1. The resin system has an excellent process window for CF wet winding molding.
2. The resin system lowers curing temperature and toughens CE without losing thermal property.
3. The CF composites molded at 155 °C has high flexural strength at 230 °C.

In this study, thiol compounds (MS) were used as free radical initiators, and diallyl bisphenol A (DBA) was used as toughening agents. Their addition lowered the molding temperature and formed a toughening cross-linked structure without sacrificing heat resistance. The CE/CF composites molded at 155 °C demonstrated great potential in rocket engine casing materials.

Keywords: Cyanate resin, Heat resistance, Toughness, Carbon fiber, Wet winding process



SELF-HEALING HYDROGELS PRINTED BY PHOTOINDUCED 3D PRINTING TECHNIQUES FOR BIOMEDICAL APPLICATIONS

Maria D'Aloia^{a,b,c,*}, Ignazio Roppolo^{b,c}, Francesca Frascella^b

^aDepartment of Chemistry, Biology and Biotechnology, University of Perugia, Perugia, Italy

^bDepartment of Applied Science and Technology, Politecnico di Torino, Turin, Italy

^cCenter for Sustainable Future Technologies, Italian Institute of Technology, Turin, Italy

*maria.daloia@polito.it

Abstract

Self-healing hydrogels (SHHs) are promising materials in tissue engineering due to their ability to mimic the biomechanical properties of biological tissues and autonomously repair damage¹, and can serve as ideal three-dimensional scaffolds for cell proliferation and differentiation. However, conventional processing methods, such as extrusion-based printing, often limit the complexity and resolution of the fabricated structures. Light-induced 3D printing, particularly Digital Light Processing (DLP), on the other hand, offers advantages in terms of resolution, printing speed and design freedom³, making it an attractive approach for developing SHHs.

This study aims to develop a biocompatible and self-healing hydrogel through DLP, enhancing structural complexity while maintaining self-repairing properties. The hydrogel is made from polyethylene glycol diacrylate (PEGDA), hydroxyethyl methacrylate (HEMA), dithiothreitol (DTT) and borax, and the solvent is PBS. Crosslinking occurs by radical photopolymerization between PEGDA, HEMA and DTT, with the latter that also reacts with borax, forming boronate-ester bonds, which impart self-healing properties to the material by enabling reversible crosslinking. Complex 3D structures were fabricated using a commercial DLP printer, and self-healing properties were assessed. Chemical (FTIR, NMR), rheological, and mechanical analyses were performed, along with cytocompatibility tests. The hydrogel exhibited successful 3D printability, allowing the fabrication of complex structures. Self-healing tests demonstrated that, after 72 hours, the samples could self-repair and withstand tensile forces, maintaining their integrity after multiple damage-repair cycles. Chemical and mechanical characterization confirmed the stability and viscoelastic behaviour of the material, while preliminary cytocompatibility assays indicated suitability for tissue engineering applications.

DLP-based printing enables the fabrication of self-healing hydrogels with improved resolution and design freedom. The developed hydrogel exhibits promising mechanical properties and biocompatibility, making it a strong candidate for tissue engineering applications.

Keywords: Self-healing hydrogel; 3D printing; DLP

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PREPARATION OF STIMULI-RESPONSIVE HYDROGEL PARTICLES AND ADSORPTION/DESORPTION OF ORGANIC DYE

Hyo Takahashi^a, Masahiro Muraoka^a, Motohiro Shizuma^{a,b}, Shintaro Kawano^{b*},

^aOsaka Institute of Technology

^bOsaka Research Institute of Industrial Science and Technology

*Corresponding author: skawano@orist.jp

Abstract

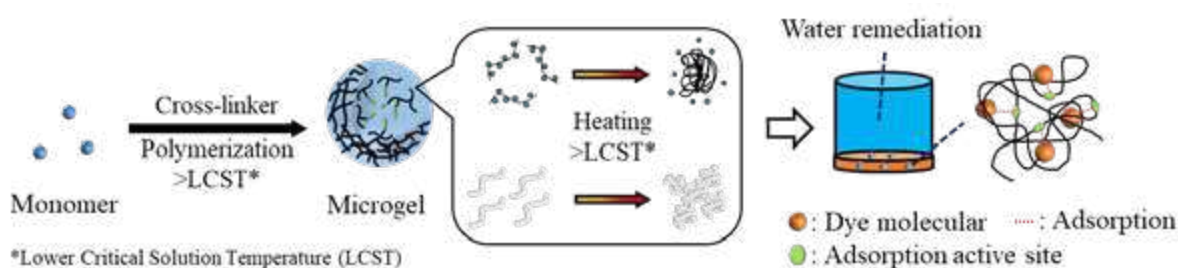
With the use of large amounts of organic dyes, e.g. industries like food, leather, paint, plastic, and textiles release effluents that significantly impact water quality, affecting both surface and underground water bodies. For example, a batik which is a piece of woven cloth decorated with patterns and designs is colored by organic dyes such as acid dye (e.g. Acid Orange 20).¹ Wastewater containing many dyes and chemicals can harm the environment and cause health risks. Therefore, treatments of batik effluent including acid dye are very crucial and the removal of color is a major challenge.

Although microgels are effective adsorbents for removing organic dyes from water effluents, the separation of the adsorbates and remediated water from the wastewater presents significant challenges.² Due to the soft and swollen nature of these materials, they tend to remain water soluble, making them difficult to recover from the system. Therefore, it is crucial points to convert to insoluble stuffs with more hydrophobic aggregation or flocculation state in water. In our study, we have been focusing on cross-linked hydrogels and/or particles using stimuli-responsive polymers whose properties change in response to external environment such as temperature and pH values. Here, we present our method to stably form insoluble microgels, their use as dye adsorbents, and their desorption function for material recycling.

1. Preparation of thermo- and pH-responsive hydrogel particles which can disperse in water.
2. Study of isotherm adsorption and the adsorption kinetics for Acid Orange 20 using hydrogel particles to evaluate the removal efficiency and adsorption capacity.³
3. Recovery of adsorbents by desorption of dye and characterization of desorption efficiency.

We will present the results, achieving higher removal efficiency of Acid Orange20, recovery and recycle use of the adsorbents by dye desorption using hydrogel particles.

Keywords: stimuli-responsive polymers, microgels, adsorption and desorption, organic dyes



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PHOTOCURABLE POLYMERS AND THEIR INTERACTION WITH TERAHERTZ RADIATION: A PATHWAY TO 4D PRINTABLE POLYMERIC META-DEVICES FOR 6G TECHNOLOGIES

Beatrice Tosetto^{1,2,3,*}, Fabrizio Candido Pirri^{1,3}, Giancarlo Rizza⁴, Ignazio Roppolo^{1,3}

¹Department of Applied Science and Technology, Politecnico di Torino, Torino 10129, Italy, ²Department of Chemistry, Biology and Biotechnology, University of Perugia, 06123, Perugia, Italy, ³Center for Sustainable Future Technologies, Italian Institute of Technology, 10144 Turin, Italy, ⁴Laboratoire des Solides Irradiés, CEA/DRF/IRAMIS, Institut Polytechnique de Paris, CNRS, Palaiseau 91128, France

*beatrice.tosetto@polito.it

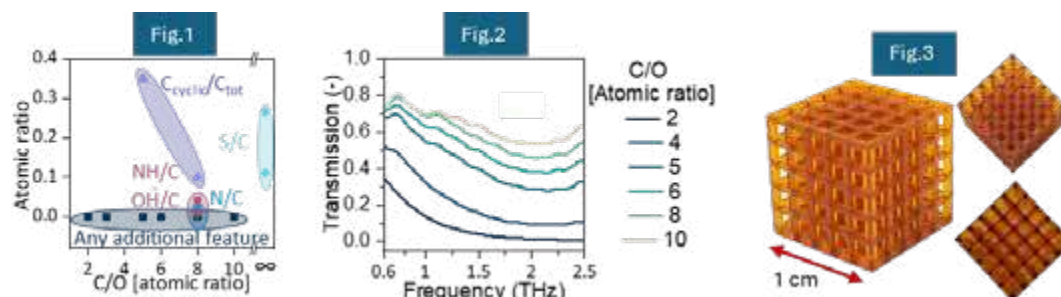
Abstract

The next generation of wireless communication (6G), foreseen for the 2030s, will be based on terahertz (THz) radiation. 6G is predicted to aggregate multiple resources, becoming a digital ecosystem that connects the digital, physical, and human worlds.¹ Beyond 6G, THz frequencies are also gaining interest in many applications in different areas, such as biomedical, quality control, security, and defense.²

In this work, the possibility of creating a stimuli-responsive metamaterial that can interact with THz in a programmable and controlled way was investigated to develop 4D printable sensors for THz radiation. This was possible by exploiting polymeric material characteristics and combining them with pattern designs, and responsive dyes.

Despite the pivotal role that this part of the electromagnetic spectrum will play in the next future, the knowledge on matter/radiation interaction is lacking, especially for polymeric materials. To address this, THz-time domain spectroscopy on various photocured (meth)acrylates and thiol-ene resins with different chemical compositions (Fig.1) were conducted, evidencing a precise relationship between the present bonds and the THz transmission (Fig.2). The definition of this dataset was the cornerstone to design new formulations that could meet the transparency criteria request for the development of THz-active metastructure. Those metamaterials have user-defined interaction with THz radiation thanks to specific pattern designs with geometric features of hundreds of microns, and those characteristics are perfectly compatible with 3D printing capabilities, particularly with Digital Light Processing technology, the one used for this work.³ Finally, the integration of photoresponsive AZO-compounds within the printed formulation allowed to obtain high printing resolution (Fig.3) and, additionally, the possibility to trigger a modulation of the radiation transmission, resulting in a THz-active 4D printed metamaterial with a light-controlled THz interaction. These findings open new perspectives for the advanced manufacturing of multifunctional polymeric materials in strategic fields such as electronics and telecommunications.

Keywords: Photopolymerization, photoresponsivity, stimuli-responsive, Terahertz, 4D Printing



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UV-BARRIER POLY(LACTIC ACID) FILM WITH LIGHT-STABILISED EU COMPLEXES AS FILLER

Linze Liu^a, Tungalag Dong^a, Lijun Song^b, Xueyan Yun^{a*}

^a College of Food Science and Engineering, Inner Mongolia Agricultural University

^b Xiamen Key Laboratory of Rare Earth Photoelectric Functional Materials, Xiamen Institute of Rare Earth Materials, Chinese Academy of Sciences

*Corresponding author: yun_imau@163.com

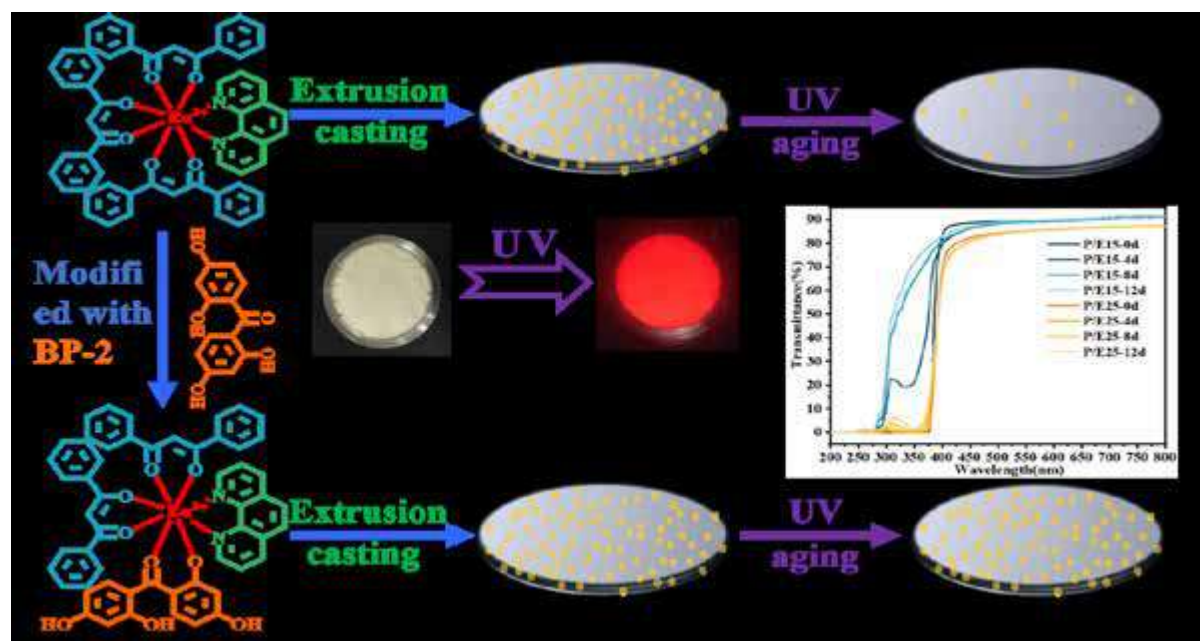
Abstract

The poor UV shielding property of PLA limit it further applications on food packaging. The rare-earth complex Eu(DBM)₃phen converts absorbed ultraviolet (UV) light to red light, which inspires the development of new UV shielding materials. However, this complex has low photostability and decomposes easily under UV irradiation. Thus, we prepared a long-lasting rare-earth complex transluinant Eu(DBM)₂(BP-2)phen by introducing BP-2 into Eu(DBM)₃phen, and blended it with PLA to obtain PLA/Eu(DBM)₂(BP-2)phen composite films. Herein discussion will be focused on the following points with the goal of enhancing the UV barrier performance of PLA.

1. A long acting rare earth light transfer agent was synthesized, which could provide long-term UV shielding performance for PLA.
2. The effects of UV aging on the properties of PLA-based barrier films were studied.
3. The PLA-based UV barrier films was used to protect flaxseed oil.

As a result, the film had long-lasting UV shielding performance, good transparency and mechanical properties. Finally, the film was used to retarded the oxidation process of the oil.

Keywords: UV shielding; PLA; Eu(DBM)₂(BP-2)phen; packaging; rare-earth complex



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A STUDY ON THE DURABILITY OF METAL-COMPOSITE HYBRID JOINTS FABRICATED USING INSERT INJECTION MOLDING IN AUTOMOTIVE DRIVING ENVIRONMENTS

Yeong-won Lim^a, Younki Ko^a, Jinho Park^{a*}

^aKorea Automotive Technology Institute

*Corresponding author: parkjh1@katech.re.kr

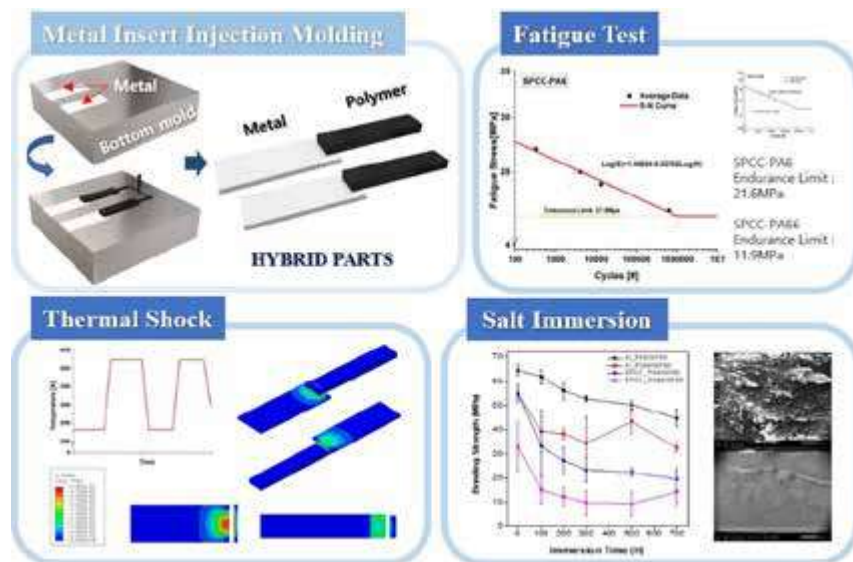
Abstract

In the automotive industry, lightweight has been the most important challenge. The recent expansion of electric vehicle production and demand has raised issues, but these are not problems unique to electric vehicles. Lightweighting improves fuel efficiency, acceleration, and performance at braking distances, as well as exhaust emissions. As a solution, research on metal-polymer hybrid automotive parts is actively being conducted. In order to apply it to vehicles, it is also essential to evaluate the durability of components in the driving environment.

In this study, specimens were prepared by insert injection molding using glass fiber reinforced PA6, PA66, and SPCC as main materials. The material properties were confirmed by glass fiber content, and durability tests were conducted on metal-polymer heterojunction specimens manufactured by insert injection molding.¹ In consideration of the driving environment and vehicle interior environment, repeated thermal shock tests and salt immersion tests were conducted.² In addition, the fatigue test revealed the long-term performance.

As a result, thermal stress generated during thermal shock test causes natural fracture at metal-polymer interface. The longer the immersion time of the salt immersion test increased, the lower the durability. The fatigue test also confirmed that PA6 is more suitable for hybrid parts than PA66. Prior to application to automobile parts, the expected life of the metal-polymer hybrid bonding was confirmed through various internal environmental tests.

Keywords: Metal-Composite, insert injection, hybrid bonding, durability, environmental test



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LOW DARK CURRENT ORGANIC X-RAY SENSORS BASED ON A MEDIUM BANDGAP POLYMER DONOR

Hye-Seong Ko^a, Jong-Woon Ha^b, Do-Hoon Hwang^{a*}

^aPusan National University.

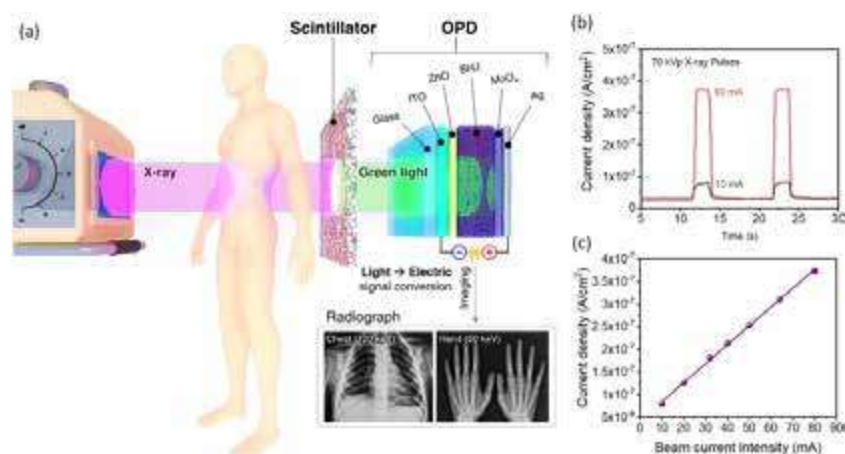
^bGyeongsang National University.

*Corresponding author: dohoonhwang@pusan.ac.kr

Abstract

In this study, we present the development of an organic X-ray image sensor utilizing a medium bandgap polymer donor with low dark current, aiming to enhance the performance and practicality of X-ray detection systems. Conventional X-ray detectors, which rely on silicon-based photodetectors coupled with scintillators, suffer from significant limitations such as high weight, rigidity, and fabrication complexity, making them less suitable for portable or flexible imaging applications. To overcome these challenges, we designed and implemented a bithienopyrrolodione-based polymer donor, which enables the fabrication of a thick active layer (~700 nm) while maintaining excellent photodetection properties. The proposed device exhibits a high responsivity of 0.29 A/W and an extremely low dark current density of approximately 10^{-10} A cm⁻² under a reverse bias of -2.0 V. These characteristics contribute to an improved signal-to-noise ratio and high specific detectivity, ensuring enhanced imaging performance. Our findings demonstrate the potential of organic photodetectors for next-generation X-ray imaging sensors, particularly in applications requiring lightweight, flexible, and portable detection systems.

Keywords: Organic X-ray Image Sensors, Conjugated Polymer Donor, Organic Photodetector, Low Dark Current



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SOL-GEL POLYMERIZATION OF MOLECULARLY IMPRINTED O-CRESOL: PREPARATION, CHARACTERIZATION AND APPLICATION

Mohamad Raizul Zinalibdin^{a,*}, Norshahida Samsuri^a, Ahamad Huzairan Abdul Ghafar^a,
 Suriani Mat Yassin^a,

^aDepartment Chemistry of Malaysia Petaling Jaya

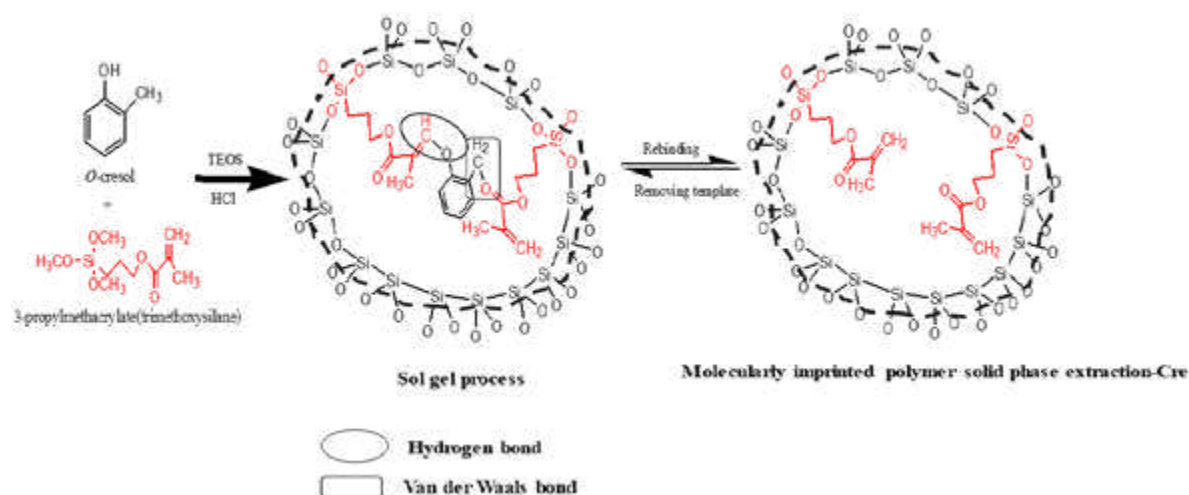
*Corresponding author: mohdraizul@kimia.gov.my

Abstract

In this study, a novel o-cresol molecularly imprinted polymer (MIP) composite was synthesized via sol-gel polymerization. o-Cresol, a metabolite of toluene, was selected as the template molecule, while 3-propyl(methacrylate)trimethoxysilane (3-PMTMOS) served as the functional monomer, tetraethoxysilane (TEOS) as the cross-linker, and ethanol as the porogenic solvent. The synthesized MIP and its non-imprinted counterpart (NIP) were characterized using Fourier transform infrared (FTIR) spectroscopy, nitrogen adsorption analysis for textural properties, and field emission scanning electron microscopy-energy dispersive X-ray (FESEM-EDX). The MIP synthesized with 800 μ L of 3-PMTMOS, 12 mL of ethanol, 12 mL of TEOS, 0.05 mmol of o-cresol, and 400 μ L of hydrochloric acid demonstrated the highest adsorption capacity (0.99 mg/g) and an enhanced imprinting factor (IF) of 4.95. This MIP was employed as an adsorbent for the extraction of o-cresol from urine samples, enabling the monitoring of occupational toluene exposure in workers.

Keywords: o-Cresol, Toluene metabolite, Molecularly Imprinted Polymer, Sol-gel Polymerization.

Graphic / Image



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INNOVATIVE INTELLIGENT FOOD PACKAGING INCORPORATING κ -CARRAGEENAN/POLYANILINE FILMS

Kar Yan-Fong^a, Ishak Ahmad^b, Sook Wai-Phang^{a*}

^a*Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology (TARUMT), 53300, Setapak, Kuala Lumpur, Malaysia.*

^b*Polymer Research Centre (PORCE), Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600, Bangi, Selangor Darul Ehsan, Malaysia.*

**Corresponding author: phangsw@tarc.edu.my*

Abstract

Intelligent food packaging has been designed to overcome significant global food waste issues, with reports showing that 19% of food production is wasted in households and food services. Natural colourants and chemical chromogenic methods have been widely applied for food freshness monitoring through colour changes. However, these approaches may pose the risk of chemical reagent migration to food and exhibit low sensitivity. Polyaniline (PANI), with its unique properties of exhibiting different colours at various oxidation states, has emerged as a promising alternative. In this study, PANI was synthesized through the chemical oxidative method and incorporated into kappa-carrageenan (κ -CGN) to develop intelligent food packaging labels for ammonia detection. Both PANI and κ -CGN/PANI films were characterised using FTIR, UV-Vis and low resistivity meter for chemical structure and oxidation state confirmation, while TGA analysis and tensile testing were conducted on κ -CGN/PANI films to evaluate their thermal stability and mechanical properties as intelligent food packaging. The indicator performance was studied with ammonia concentrations ranging from 200 - 1000 ppm and temperatures from -20°C - 40°C, where a colour change from green to blue was observed within 45 minutes. κ -CGN/PANI 0.50% showed optimal performance, with a high sensitivity of 0.00005, strong linearity ($R^2 = 0.9945$), good precision (RSD = 1.50%), and LOQ of 638 ppm. Long-term stability and real sample analyses showed consistent normalized signals, reinforcing the potential of κ -CGN/PANI films as reliable label-based freshness indicators for intelligent food packaging.

Keywords: intelligent food packaging; polyaniline; kappa-carrageenan; food freshness indicator; ammonia detection

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POLYSACCHARIDE-BASED WOUND DRESSING WITH NANOFLOWERS AS A ADVANCED BIOMATERIALS FOR WOUND THERAPY

Dorota Chelminiak-Dudkiewicz^{a*}, Miloslav Machacek^b, Klara Konecna^c, Kinga Mylkie^a, Aleksander Smolarkiewicz-Wyczachowski^a, Marta Ziegler-Borowska^a

^aDepartment of Biomedical Chemistry and Polymer Science, Faculty of Chemistry, Nicolaus Copernicus University in Torun, Gagarina 7, 87-100 Torun, Poland.

^bDepartment of Biochemical Sciences, Faculty of Pharmacy in Hradec Kralove, Charles University in Prague, Akademia Heyrovskeho 1203, 500-05 Hradec Kralove, Czech Republic.

^cDepartment of Biological and Medical Sciences, Faculty of Pharmacy in Hradec Kralove, Charles University in Prague, 9, Zborovska 208, 500 05, Hradec Kralove, Czech Republic.

*Corresponding author: dorotachd@umk.pl

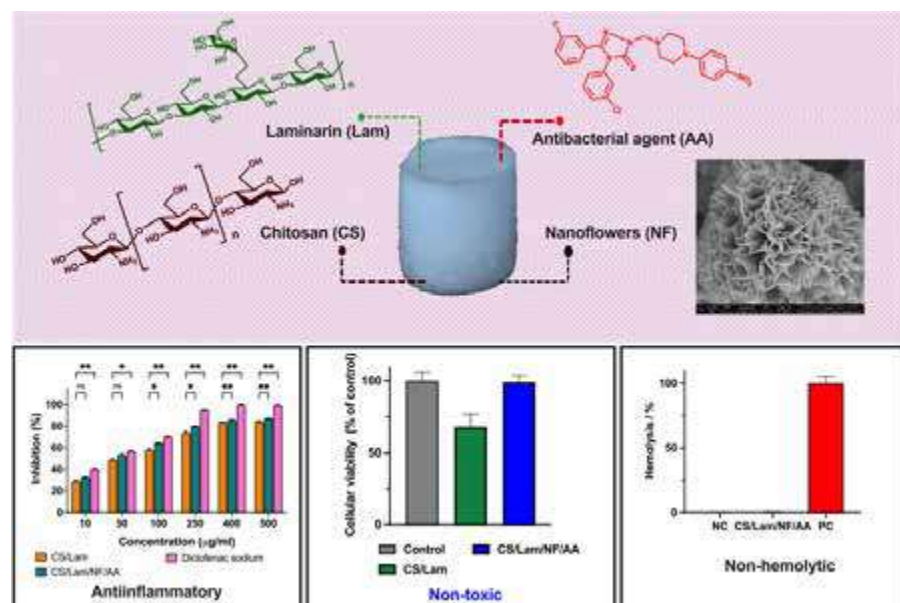
Abstract

In civilian trauma and military combat, uncontrollable post-traumatic bleeding and bacterial infections are major life-threatening factors. Poor sanitation on battlefields and poor living conditions of victims are conducive to bacterial infections. Hence, this study developed a new advanced nonpressing three-in-one dressing material using adhesive biopolymers, hybrid protein-inorganic nanoflowers, and antibacterial agent to provide effective bleeding and septic control. A mixture of chitosan and laminarin was used as the biopolymer base, while the nanoflowers were produced using the plant enzyme bromelain. Systematical characterizations of the obtained biomaterial, including surface morphology, chemical structure, thermal stability, and mechanical performance, were performed. The biological effect of the sponge was also assessed, and according to the results, the material exhibited excellent anti-inflammatory, antioxidant, and antimicrobial properties, as well as non-hemolytic material, as indicated by hemolysis tests. Furthermore, the sponges were non-toxic and compatible with MRC-5 fibroblasts. The designed sponges have conclusively proven their beneficial physicochemical properties and, at the preliminary stage, biocompatibility, and therefore, can be considered promising material for wound dressings in future *in vivo* applications.

Keywords: laminarin, bromelain, nanoflowers, wound dressing, biomaterials

Acknowledgment

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SYNTHESIS AND CHARACTERIZATION OF NANOCOMPOSITES BASED ON SPINEL FERRITE OXIDE AND POLYPYRROLE $\text{Zn}_{0.3}\text{Mg}_{0.7}\text{Fe}_2\text{O}_4$ @PPY FOR INDUSTRIAL APPLICATIONS

Modou Gningue Diop, Mamadou Gueye, Mor Cissé ; Momath Lo; *Makhtar GUENE

Laboratoire de Chimie Physique Organique et d'Analyses Environnementale Département de Chimie Faculté des Sciences et Techniques Université Cheikh Anta Diop –Dakar/ SENEGAL

**Corresponding author: makhtar.guene@ucad.edu.sn maguene@gmail.com*

Abstract :

In this study, the physico-chemical properties of ferrite spinels, a magnetic nanocomposite composed of spinel oxide ($\text{Zn}_{0.3}\text{Mg}_{0.7}\text{Fe}_2\text{O}_4$) and polypyrrole polymer (PPy), were investigated. The oxide was synthesized using sol-gel method, followed by oxidative polymerization. The structure of the compounds was studied using Raman and FT-IR spectroscopy. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were used to determine the morphology and core-shell structure, respectively. Furthermore, electrochemical studies were carried out using cyclic voltammetry (CV), which revealed that the nanocomposite is more conductive than the oxide alone. The electrochemical analysis results demonstrated that the $\text{Zn}_{0.3}\text{Mg}_{0.7}\text{Fe}_2\text{O}_4$ @PPy nanocomposites exhibited enhanced redox activity and a higher current intensity. This study highlights the development of hybrid $\text{Zn}_{0.3}\text{Mg}_{0.7}\text{Fe}_2\text{O}_4$ @PPy type nanospheres with substantial and effective electrochemical properties, which could be a suitable option for industrial applications. This work demonstrates the significance of polymers in enhancing the conductivity of ferrite spinels without modifying their configuration. Furthermore, it illustrates the possibility of constructing hybrid materials through the interaction between PPy and ferrite spinels. These ferrite spinels can be employed as a model for the in-situ electrodeposition of polypyrrole nanocomposites, which results in the formation of polymers with notable electrochemical properties.

Keywords: Ferrite spinels, polypyrrole polymer; sol-gel method; electrochemical studies; cyclic voltammetry; hybrid mixed oxides.

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MN(III) O^NO COMPLEXES AS WATER-TOLERANT AND ENVIRONMENTALLY BENIGN CATALYSTS FOR POLYURETHANE FOAM SYNTHESIS

Wei-Chieh Chang,^a Edward Ocansey,^a Oliver Sala,^b Marina Kamm,^c Maximilian Joost,^b Stefan Bokern,^c Frank Rominger,^d A. Stephen K. Hashmi,^d Thomas Schaub,^{a,b} and Jaroslaw Mormul^{a,b,*}

^aCatalysis Research Laboratory (CaRLa), University of Heidelberg, Im Neuenheimer Feld 271, 69120 Heidelberg, Germany

^bBASF SE, Carl-Bosch-Straße 38, 67056 Ludwigshafen, Germany

^cBASF Polyurethanes GmbH, Elastogranstr. 60, 49448 Lemförde, Germany

^dOrganisch-Chemisches Institut, Heidelberg University, Im Neuenheimer Feld 270, 69120 Heidelberg, Germany

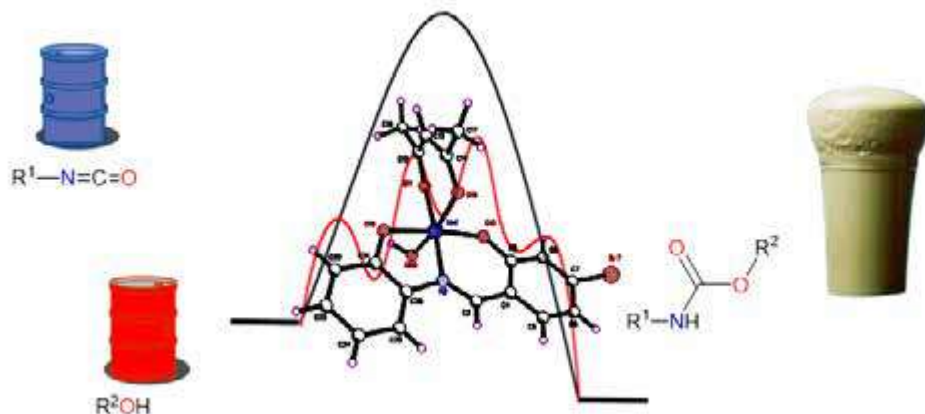
*Corresponding author: jaroslaw.mormul@basf.com

Abstract

Polyurethanes are synthesized on industrial scale by the reaction of diisocyanates with diols in the presence of catalysts which are commonly based on tin complexes and amines.^{1,2} However, due to the toxicity and volatility of these tin catalysts and amines, there is the need to develop new catalysts that are more environmentally benign.^{3,4}

Herein, we report the synthesis of O^NO pincer-ligated Mn(III) and Fe(III) complexes that serve as suitable catalysts for urethane formation and are stable to hydrolysis as predicted by computations and observed experimentally.⁵ The O^NO pincer scaffold is vital to the activity of these catalysts, simultaneously ensuring increased solubility in the reaction medium as well as providing a stable framework upon dissociation of co-ligands in the catalytic cycle. In silico mechanistic investigations for urethane formation show that the stabilization of active species in square-planar geometries enabled by these O^NO ligands permit the simultaneous coordination of alcohol and isocyanate in suitable configuration at the metal center.

Keywords: Polyurethane, PU foam, Fe & Mn catalysts, water stability, mechanisms



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DYNAMIC CROSSLINKING OF COMMODITY THERMOPLASTICS TO CREATE RECYCLABLE THERMOSETS VIA PERFLUOROPHENYL NITRENE C-H INSERTION

Zhi Yuan Lee,^a Sirin Kamarulzaman,^{a,b} Rizqullah Rasyiddin,^a Sheila Y.X. Sim,^a Georgina E.K.K. Seah,^a Ai Wei Gan,^a Zibiao Li,^{a,c,d} Zhuang Mao Png,^c and Shermin S. Goh^{a,*}

^a*Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR)*

^b*School of Materials Science and Engineering, Nanyang Technological University*

^c*Institute of Sustainability for Chemicals, Energy and Environment (ISCE2), A*STAR*

^d*Department of Materials Science and Engineering, National University of Singapore*

**Corresponding author: gohsm@imre.a-star.edu.sg*

Abstract

Covalent Adaptable Networks (CANs) represent a new class of polymers that contains dynamic covalent bonds (DCBs), granting them the recyclability of thermoplastics while retaining the superior mechanical properties and stability of thermosets^{1,2}. One approach to form CANs is by directly incorporating DCBs into the polymer backbone during the polymerization process,^{3,4} which are important for extending material service lifespan and meeting sustainability demands. However, these materials are often derived from non-renewable petrochemical feedstocks, or by multi-step modification of bio-based feedstocks. Here, we disclose a fully bio-based vitrimeric poly(acetal However, this remains challenging for crosslinking poly(olefins) due to their fully hydrocarbon backbone and low functionality. In this work, we introduced perfluorophenyl azide-based crosslinkers, containing disulfide, imine, and acetal DCBs, to crosslink with poly(olefins) and other thermoplastics by thermal activation, transforming them into CANs.⁵ During the crosslinking process, the perfluorophenyl azide groups generate reactive nitrene species, which subsequently insert into C-H bonds within the thermoplastics, forming permanent -NH-C- linkages. The synthesized CANs exhibited dimensional and solvent stability, as well as self-healing capabilities. Multiple cycles of chemical and/or mechanical recycling could be performed due to the exchange of DCBs. Furthermore, existing or postconsumer plastics could serve as starting materials in this crosslinking approach, with the added benefits of enhancing their thermomechanical properties and ensuring the closed-loop recyclability of these polymers.

Keywords: covalent adaptable networks, vitrimers, C-H functionalization, dynamic covalent bonds, perfluorophenyl azide

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EFFICIENT NEAR-INFRARED UPCONVERSION ORGANIC LIGHT-EMITTING DIODES

Yingli Shi^{a,*}, Yun Hu^b

^aDepartment of Electrical and Electronic Engineering, Xi'an Jiaotong-Liverpool University, Suzhou, Jiangsu, 215123, P. R. China

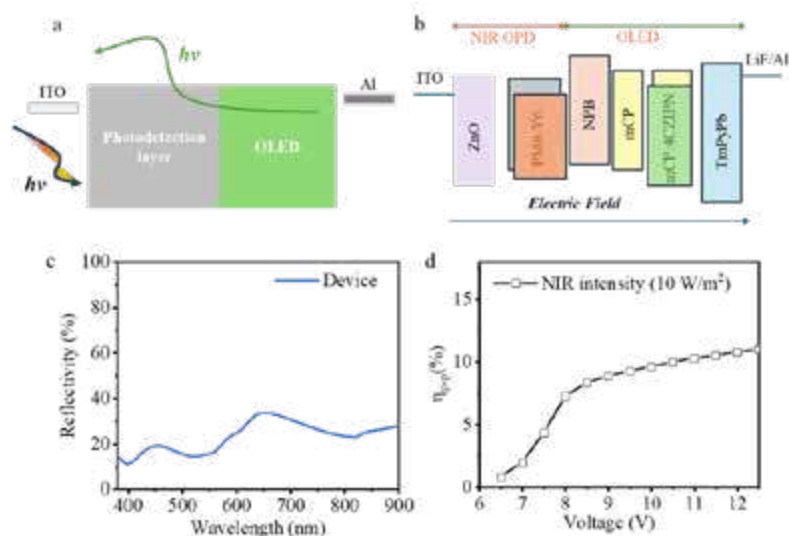
^bSuzhou Laboratory, Suzhou, Jiangsu, 215100, P. R. China

*Corresponding author: Yingli.shi@xjtlu.edu.cn

Abstract

Optical upconverters that transform near-infrared (NIR) light into visible light by directly integrating organic photovoltaic (OPV) devices with organic light-emitting diodes (OLEDs) in series are gaining significant attention for their potential applications in medicine, night vision, security, and detection.¹⁻³ The utilization of organic materials eliminates the dependency on NIR Si integrated circuits and removes constraints on substrate types. The superior performance of organic compounds, combined with the manufacturing flexibility of OLEDs, streamlines the production process and reduces costs. The color of the upconversion electroluminescence spectrum can be tuned across the visible region, ranging from blue to red. We introduce all-organic, full-color upconversion devices that integrate thermally activated delayed fluorescence (TADF)-OLEDs with NIR-sensitive bulk heterojunctions. These devices are capable of directly emitting visible light in response to incoming NIR illumination without the need for interconnected electronics or additional external displays. Typically, an increase in near-infrared irradiation intensity enhances device emission brightness; however, performance tends to be suboptimal under low infrared radiation conditions. Therefore, improving device performance under low irradiance is a critical focus of our research. Our device achieved a maximum luminance exceeding 100 cd/m² of green light at a bias of 8.5 V when illuminated by an 840 nm NIR LED (1 mW/cm²), and attained an infrared-to-visible upconversion efficiency of 7.23%.

Keywords: organic materials, upconversion, near infrared, organic light-emitting diode



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DEVELOPMENT OF IONIC-CONDUCTIVE HYDROGELS FOR WEARABLE SENSORS: EXPLORING CATION EFFECTS AND THEIR IMPACT ON PERFORMANCE

Mei-Yu Yeh^{a,*}, Dian-Huan Ji^a

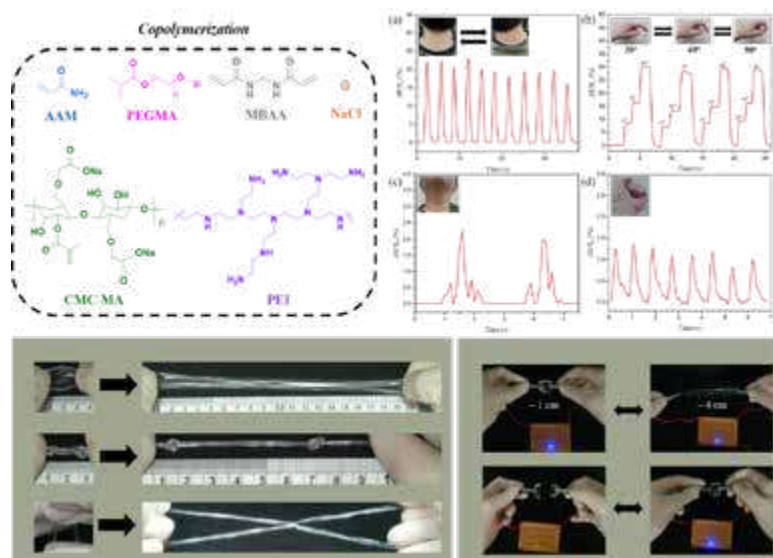
^aDepartment of Chemistry, Chung Yuan Christian University

*Corresponding author: myyeh@cycu.edu.tw

Abstract

Hydrogels are widely employed in biomedical applications due to their outstanding properties, including biocompatibility, high water content, flexibility, and elasticity. In particular, conductive hydrogels, which uniquely integrate electrical conductivity with mechanical flexibility, have gained attention as essential materials for advanced flexible and wearable sensors. Despite significant advancements in hydrogel research, designing an adhesive hydrogel that simultaneously achieves high stretchability, fatigue resistance, and reversible adhesion remains a major challenge. In this study, we aimed to develop a cost-effective, easily manufacturable hydrogel sensor utilizing ionic compounds as the primary source of conductivity. The hydrogels were synthesized using acrylamide, *N,N'*-methylenebis(acrylamide), chemically modified poly(ethylene glycol), and carboxymethyl cellulose, achieving an impressive adhesive strength of 717.2 kPa on glass surfaces.¹ Building upon this formulation, polyethylenimine was incorporated, and systematic variations of LiCl, NaCl, and KCl were introduced to examine their effects on the hydrogel's nanostructure and mechanical behavior. These formulations were designated as Li-CH, Na-CH, and K-CH, respectively. Among the tested formulations, Na-CH exhibited superior performance, demonstrating optimized elongation at break, tensile strength, and toughness, emphasizing the critical role of ion selection in hydrogel design. Additionally, Na-CH showcased remarkable stretchability, high optical transparency, and exceptional sensitivity in detecting a broad range of body movements, from large-scale gestures to subtle physiological signals such as pulse monitoring.² With its unique combination of mechanical robustness, optical clarity, and reliable sensing capabilities, Na-CH presents significant potential for applications in flexible electronics, healthcare monitoring systems, and next-generation smart display technologies.³

Keywords: conductive hydrogel, ionic compound, adhesive, stretchability, wearable sensors



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CHIRALITY-GUIDED DESIGN AND SELF-ASSEMBLY OF SUPRAMOLECULAR HYDROGELS

Hsin-Chieh Lin^{a,*}

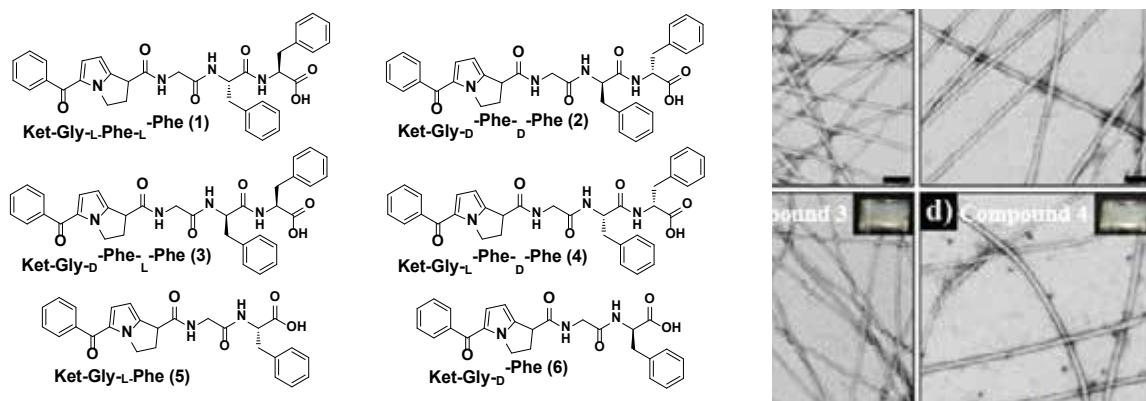
^a Department of Materials Science and Engineering, National Yang Ming Chiao Tung University

*Corresponding author: hclin45@nycu.edu.tw

Abstract

Supramolecular hydrogels, formed via the self-assembly of small molecules in water, have gained attention as versatile soft nanomaterials.^{1,2} Due to their non-covalent interactions, they naturally exhibit biocompatibility and biodegradability, making them ideal for self-delivery therapies where the drug itself serves as the hydrogelator. Unlike polymer-based drug delivery systems, supramolecular hydrogels avoid issues like inflammation and limited drug-loading capacity. Here, we design and synthesize hydrogelators derived from amino acids and Ketorolac (Ket), a nonsteroidal anti-inflammatory drug, to develop multifunctional supramolecular hydrogels with enhanced cyclooxygenase-2 (COX-2) selectivity. A series of amphiphilic Ket-capped peptides were synthesized, including Ket-Gly-L-Phe-L-Phe, Ket-Gly-D-Phe-D-Phe, Ket-Gly-D-Phe-L-Phe, Ket-Gly-L-Phe-D-Phe, Ket-Gly-L-Phe, and Ket-Gly-D-Phe. Among them, only the Ket-capped tripeptide can self-assemble in aqueous solutions, forming supramolecular hydrogels at physiological pH (pH 7.0). We confirmed their self-assembly mechanism and hydrogel behavior using UV-vis absorption spectroscopy, circular dichroism, fluorescence spectroscopy, Fourier transform infrared spectroscopy, transmission electron microscopy, and rheometry. Notably, Ket-Gly-D-Phe-D-Phe exhibited a significantly higher COX-2/COX-1 selectivity ratio of 5.8, compared to Ketorolac and other Ket-peptides, which had ratios below 1. This highlights the critical role of chirality in enzyme selectivity, as the D-Phe-D-Phe configuration enhances COX-2 binding while reducing COX-1 interaction. These findings suggest that the supramolecular hydrogels of Ket-Gly-D-Phe-D-Phe hold promise for localized, sustained-release applications. By minimizing systemic toxicity and enhancing therapeutic efficacy, this approach offers a novel hydrogel design strategy for safer and more effective anti-inflammatory therapeutics.

Keywords: Amphiphilic peptide, ketorolac, self-assembly, supramolecular hydrogel, chirality



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SUSTAINABLE SURFACTANT-MODIFIED MONTMORILLONITE: A PLANT-BASED ALTERNATIVE TO CONVENTIONAL ORGANOCLOYS

Nur Aliaa Zulkefli^{a*}, Mohd Aidil Adhha Abdullah^a, Mazidah Mamat^a, Mohamad Khairi Mohd Zainol^b, Norizah binti Mhd Sarbon^b and Azlin Fazlina bt Osman^c

^a Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030 Kuala Terengganu, Terengganu.

^b Faculty of Fisheries and Food Science, Universiti Malaysia Terengganu, 21030 Kuala Terengganu, Terengganu.

^c Biomedical and Nanotechnology Research Group, Center of Excellent Geopolymer and Green Technology (CEGeoTech), Universiti Malaysia Perlis (UniMAP), Arau 02600, Malaysia

*Corresponding author: nuraliaazulkefli@gmail.com

Abstract

Sodium montmorillonite (Na-MMT) is widely used as a nanofiller in polymer composites, but its hydrophilic nature limits compatibility with hydrophobic polymers. Surface modification with organic surfactants enhances dispersibility, yet conventional organoclays, such as the Cloisite series, are typically modified using surfactants derived from hydrogenated tallow, an animal-based source that may raise halal compliance concerns for food packaging applications. This study explores the modification of Na-MMT using four quaternary ammonium surfactants with varying hydrocarbon chain lengths: dodecyltrimethylammonium chloride (DTAC, C12), myristyltrimethylammonium bromide (MTAB, C14), cetyltrimethylammonium bromide (CTAB, C16), and octadecyltrimethylammonium bromide (OTAB, C18). The objective is to assess the effectiveness of plant-derived surfactants as sustainable alternatives to conventional animal-based surfactants in organoclay preparation. Modified Na-MMT samples were prepared via ion-exchange reactions at surfactant concentrations of 0.5, 1.0, 1.5, and 2.0 CEC. A series of characterization techniques were employed to examine the structural, thermal, and morphological properties of surfactant-modified Na-MMT. Fourier-transform infrared spectroscopy (FTIR) confirmed the successful incorporation of surfactants into the material. X-ray diffraction (XRD) demonstrated significant changes in the basal spacing of Na-MMT, with a notable increase observed when surfactants with longer hydrocarbon chains were used. CHNS elemental analysis provided quantitative data on the amount of surfactant present within the modified material. Thermogravimetric analysis (TGA) highlighted changes in thermal stability, which varied with different surfactant concentrations. The hydrophobicity of the modified Na-MMT was enhanced, as evidenced by water contact angle measurements, particularly for the CTAB- and OTAB-modified samples. Transmission electron microscopy (TEM) revealed key morphological changes, confirming successful surfactant intercalation and partial exfoliation of Na-MMT. Collectively, these analytical techniques offered a thorough understanding of the modifications and their impact on the physical and chemical properties of the material. This study demonstrates that plant-derived surfactants, particularly MTAB and CTAB, effectively modify Na-MMT, offering a viable alternative to animal-based organoclays. Their use in nanocomposite applications enhances consumer inclusivity while maintaining functional performance, making them promising candidates for sustainable food packaging solutions.

Keywords: Montmorillonite (MMT), Plant-derived surfactants, Organoclay modification, Hydrophobicity, Food Packaging

COMPARISON OF NANOCELLULOSE EXTRACTED FROM OIL PALM MESOCARP FIBRE USING ACID HYDROLYSIS AND TEMPO OXIDATION METHODS

Jo Sze Lean^{a*}, Ng Jeck Fei^{a*}, Siau Hui Mah^b, Chai Yee Chin^a, Harrison Lik Nang Lau^c,
Soek Sin Teh^c

^a School of Pharmacy, Faculty of Health and Medical Sciences, Taylor's University, 47500 Subang Jaya, Selangor, Malaysia.

^b School of Biosciences, Faculty of Health and Medical Sciences, Taylor's University, 47500 Subang Jaya, Selangor, Malaysia.

^c Energy and Environment Unit, Engineering and Processing Division, Malaysian Palm Oil Board, Selangor, Malaysia.

*Corresponding author: JeckFei.Ng@taylors.edu.my

Abstract

Oil Palm Mesocarp Fibre (OPMF), a biomass residue obtained from palm oil extraction from oil palm fruits, can be a viable source of nanocellulose (NC) as it is rich in lignocellulose. In this study, NC was synthesised from OPMF with varying surface functional groups and degrees of substitution using H₂SO₄ and HCl acid hydrolysis and TEMPO oxidation methods, and by varying H₂SO₄ acid concentration, and volume oxidising agent, NaOCl. The findings show that the NCs synthesised using the different methods resulted in NCs with different zeta potential, functional groups, sulfur and carboxylate content, thermal stability, crystallinity, and structure. DLS characterisation of the TEMPO-oxidised NCs showed that they had a higher zeta potential of -55.90 ± 1.00 mV to 66.40 ± 2.20 mV compared to 23.00 ± 1.56 mV to 29.20 ± 4.27 mV for H₂SO₄ and 23.20 ± 3.32 to 24.57 ± 2.59 mV for HCl. Moreover, TGA analysis of the NCs reveals that TEMPO-oxidised and HCl-hydrolysed NCs have higher thermal stability than H₂SO₄-hydrolysed NCs. FT-IR analysis also revealed that the H₂SO₄-hydrolysed NCs have a sulfated functional group at around 1100 cm⁻¹, and TEMPO-oxidised NCs have carboxyl functional groups at around 1420 cm⁻¹ while there is no difference for HCl-hydrolysed NCs compared to cellulose. The results from the conductometric titrations reveal that increasing concentrations of H₂SO₄ and NaOCl increased the content of sulfur and carboxylate, respectively. XRD analysis showed that the synthesised NCs have more crystallinity than cellulose. TEM analysis revealed that the TEMPO-oxidised NCs have a fibre-like appearance while the acid-hydrolysed NCs have a needle-like crystalline structure. All synthesised NCs have diameters of less than 10 nm. So far, the study found that it is achievable to synthesise NCs with different surface modifications, which can be used to formulate wound-healing nanocomposite hydrogels with good physicochemical properties.

Keywords: Oil Palm Mesocarp Fibre, nanocellulose, surface functional group, TEMPO-oxidation, acid hydrolysis

DEVELOPMENT OF A PAPER-BASED MICROFLUIDIC DEVICE FOR COLORIMETRIC DETECTION OF LEAD IONS

Sopharen Houn^a, Veasna Soum^{a,*}

^a*Graduate School of Science, Royal University of Phnom Penh.*

**Corresponding author: soum.veasna@rupp.edu.kh*

Abstract

Pb(II) is widely used, food and water are typically polluted with this dangerous element. The Environmental Protection Agency (EPA) has set a maximum acceptable limit of 10 ppb, as per the World Health Organization (WHO) and the United States government. In agreement with several epidemiological reports have recommended high lead levels in humans with a variety of diseases and disorders, including heart disease, hypertension, renal function impairment, and cancer. There are several existing methods for determining lead ions such as flame atomic absorption spectrometry (FAAS), electrothermal atomic absorption spectrometry (ETAAS), graphite furnace atomic absorption spectrometry (GFAAS), inductively coupled plasma mass spectrometry (ICP-MS), high-performance liquid chromatography (HPLC), and inductively coupled plasma optical emission spectroscopy, however, those methods required high cost and difficult to perform the detection onsite. A Microfluidic paper-based analytical device (μ PAD) is a simple and low-cost analytical device capable of heavy metals including lead. In this present research, we develop a portable μ PAD for colorimetric lead detection in liquid samples. The device consists of five layers. The first layer is a hydrophobic substrate. The second layer is Whatman no.4 filter paper, marked with a Zebra brand pen to create a detection zone with dimensions of 11.5 mm. The third and fourth layers are photo paper and adhesive plastic film, forming a hydrophobic barrier with a length of 20 mm and a reagent zone with a diameter of 5.5 mm. The fifth layer is adhesive plastic film, which serves as the cover for the device. The reagent used for lead ion detection is based on the color development of the lead rhodizonate complex on the filter paper. This device system, characterized by paper and adhesive plastic film, was successfully applied for lead ion detection. As a result, the microfluidic paper-based device can analyze lead metal concentrations using the colorimetric method, effectively analyzing standard lead solutions at concentrations ranging from 0 to 10 ppm.

Keywords: Paper-based Microfluidic, Colorimetric method, Lead ion

PHASE BEHAVIOR MODULATION OF LAMELLAR SURFACTANT AGGREGATES FOR SURFACE MODIFICATIONS

Rui A. Gonçalves^{a,*}

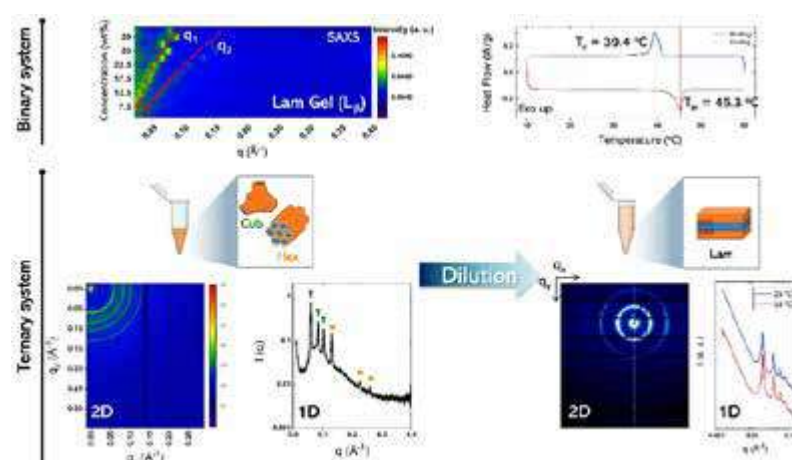
^a*School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore.*

**Corresponding author: rui.goncalves@ntu.edu.sg*

Abstract

The phase behavior of aqueous surfactant systems, particularly the transition between gel (L_β) and liquid-crystalline (L_α) phases, is sensitive to low molecular weight additives, offering a means to control surfactant solution properties [1-3]. We developed dioctadecyldimethylammonium chloride (DODAC) formulations that self-assemble into lamellar phases, transitioning between L_β and L_α depending on temperature and specific water-soluble additives. This enables tuning of the gel-to-liquid crystalline phase transition temperature (T_m), facilitating controlled deposition of lamellar structures onto surfaces [4]. In-situ null ellipsometry tracked the deposition of diluted surfactant L_β phases as the bulk solution was replaced with deionized water, allowing real-time monitoring of layer thickness and adsorption. Neutron reflectometry provided additional insights into the composition and thickness of the adsorbed layers, revealing the role of water and additives in the deposition mechanism. Our findings highlight the fine-tuning of surfactant phase transitions and surface deposition through additive control. After dilution, surfactant bilayers irreversibly adsorbed onto hydrophilic silica surfaces, forming at least one bilayer. In summary, our study provides critical insights into the molecular structure and dynamics of lamellar gel films, offering new strategies for surface deposition and colloidal stability. These results suggest potential applications in consumer care, petrochemicals, and food science, where controlled surface deposition is essential.

Keywords: Gel phase, liquid-crystalline phase, self-assembly, deposition mechanism, adsorption



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PREDICTION ON STRUCTURAL PROPERTIES AND CO₂ SOLUBILITY IN MIL-88@PEO AS THIN MIXED MATRIX MEMBRANE USING MD SIMULATION

Mohamad Adil Iman Ishak^{a,*}, Khairulazhar Jumbri^a,

^a Fundamental and Applied Sciences Department, Universiti Teknologi PETRONAS, 32610 Bandar Seri Iskandar, Perak, Malaysia.

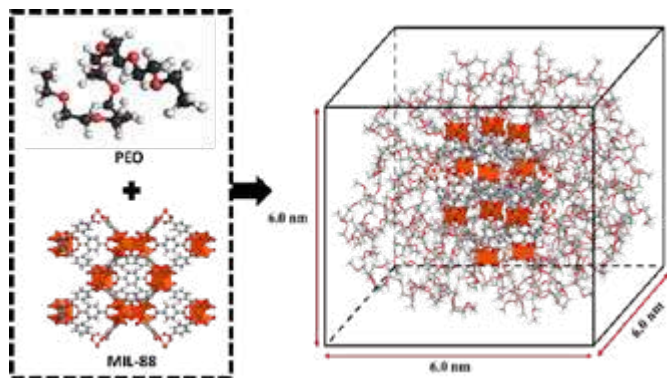
*Corresponding author: mohamad_17008596@utp.edu.my

Abstract

Membrane-based gas separation technology is one of the most promising and energy-efficient approaches for capturing excess CO₂ emissions. It offers several advantages, including low equipment cost, ease of operation, and scalability, making it a viable alternative to conventional separation techniques.^{1,2} This study presents a comprehensive molecular dynamics (MD) simulation of a mixed matrix membrane composed of MIL-88 and polyethylene oxide (PEO) for CO₂ separation. The objective is to evaluate the membrane's stability, flexibility, and CO₂ solubility using a systematic approach, including force field validation, root mean square deviation (RMSD) analysis, root mean square fluctuation (RMSF) analysis, and solvation free energy calculations. The force field validation was successful, with less than 5% difference in key parameters such as density, molecular volume, and metal-ligand distance, confirming the reliability of the selected force field. RMSD results demonstrated that increasing MIL-88 loading enhanced the structural stability of the MIL-88@PEO membrane, while RMSF analysis revealed that MIL-88's influence on flexibility varied across different atoms in PEO polymer. Notably, the highest CO₂ solubility was achieved at 15% w/w MIL-88 loading in PEO. MD simulation was conducted using GROMACS package software where solvation free energy was computed to calculate the CO₂ solubility within the membrane. These findings highlight the potential of MIL-88 as a filler in mixed matrix membranes for efficient CO₂ separation. The study provides an early prediction of the structural properties and solubility performance of the membrane, serving as a preliminary screening step before conducting experimental work.

Keywords: Molecular dynamics; metal organic framework; MIL-88; PEO; CO₂.

Graphic / Image



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BIO-BASED SUPRAMOLECULAR PHOTOCROMIC COATING

Yuting Tian^a, Guodong Fu^{a*}

^a School of Chemistry and Chemical Engineering, Southeast University

*Corresponding author: 101010855@seu.edu.cn

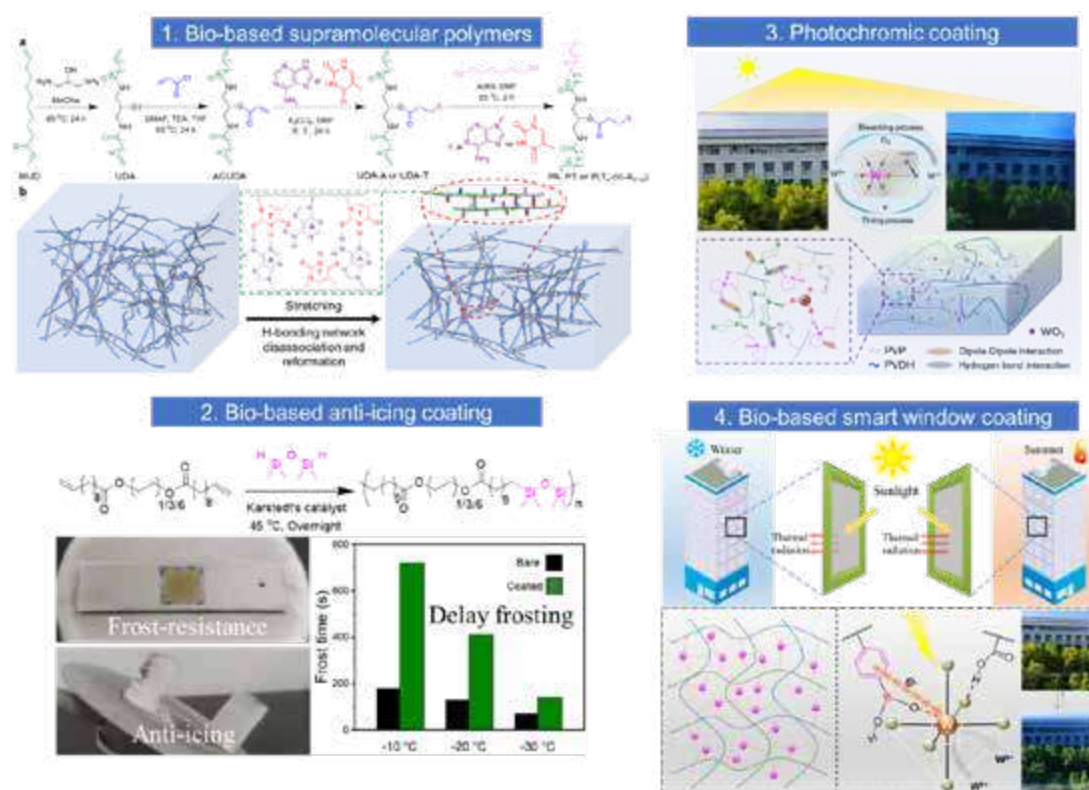
Abstract

Facing the depletion of fossil resources and global climate challenges, the development of novel materials integrating environmental sustainability, high performance, and intelligent light-response is imperative. We propose an innovative strategy based on bio-based template polymers that are synergistically designed by supramolecular interactions and photochromic technology, which is expected to prepare photochromic smart window coating with high transparency, ultra-high adhesion strength, wide dimming capability and reversible cycling stability, providing new ideas for energy-efficient buildings and sustainable development. This approach aims to provide new insights for advancing energy-efficient buildings and sustainable development.

1. Bio-based template Polymer Substrates and Supramolecular Network Construction¹
2. Multifunctional expansion²
3. Efficient integration of photochromic functions³

Multifunctional photochromic coating prepared by supramolecular engineering fused with bio-based materials break through the limitations of traditional materials and have significant potential in energy-efficient buildings and extreme protection.

Keywords: bio-based polymers, supramolecular chemistry, photochromic coating, energy conservation



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SUNLIGHT-DRIVEN GREEN APPROACHES TO CONSTRUCT DEGRADABLE HYDROGEL-BASED WEARABLE SENSORS

Jun Hu ^a, Guo-dong Fu ^{a*}

^a School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, P. R. China.

*Corresponding author: fu7352@seu.edu.cn

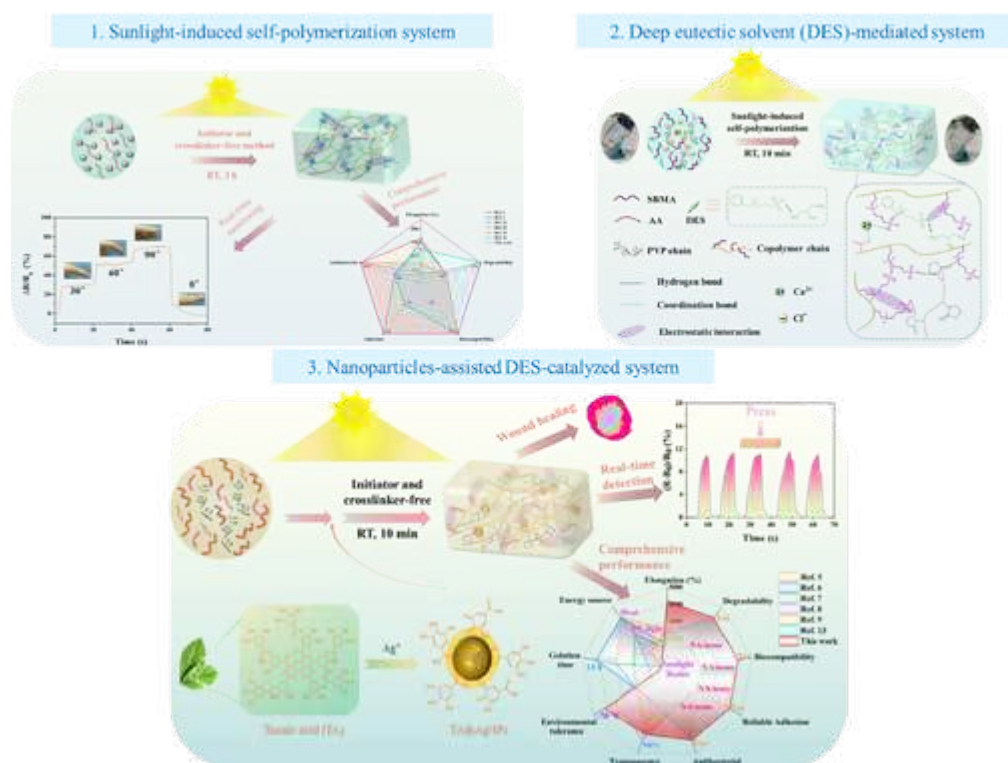
Abstract

Conductive hydrogels (CHs) are of great prospect in the field of flexible wearable electronics due to their tissue-like softness. However, current CHs have several noteworthy drawbacks, such as time-consuming processes, toxic initiator use, single function, poor degradability and self-healing performance, severely limiting their practical application. To address these challenges, we proposed a green and efficient system for preparing CHs, their rapid gelation can be triggered by sunlight, eliminating the need for external initiators or crosslinkers, the resulting hydrogels were demonstrated to be suitable for degradable wearable sensors. Through our continuous development of the sunlight-driven polymerization system, the gelation and functionality of CHs become more efficient and multiple.

1. Sunlight-induced self-polymerization system ¹
2. Deep eutectic solvent (DES)-mediated system ²
3. Nanoparticles-assisted DES-catalyzed system ³

In brief, we have put forward a series of promising avenues for constructing eco-friendly, versatile and degradable conductive hydrogels, revolutionizing the insight of wearable electronics which can accurately monitor human daily strain, voice, and deformation in real time.

Keywords: Conductive hydrogels; Flexible wearable electronics; Sunlight-driven self-polymerization; Deep eutectic solvents; Degradable



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OPTIMIZATION OF MUCILAGE EXTRACTION FROM *OPUNTIA FICUS-INDICA* FOR ECO-FRIENDLY MATERIALS

Munyadziwa B. Nemasovhani^a, Ignatia Khumalo^a, Grace Ngubeni^a, Siziwe Gqoba^{a*}

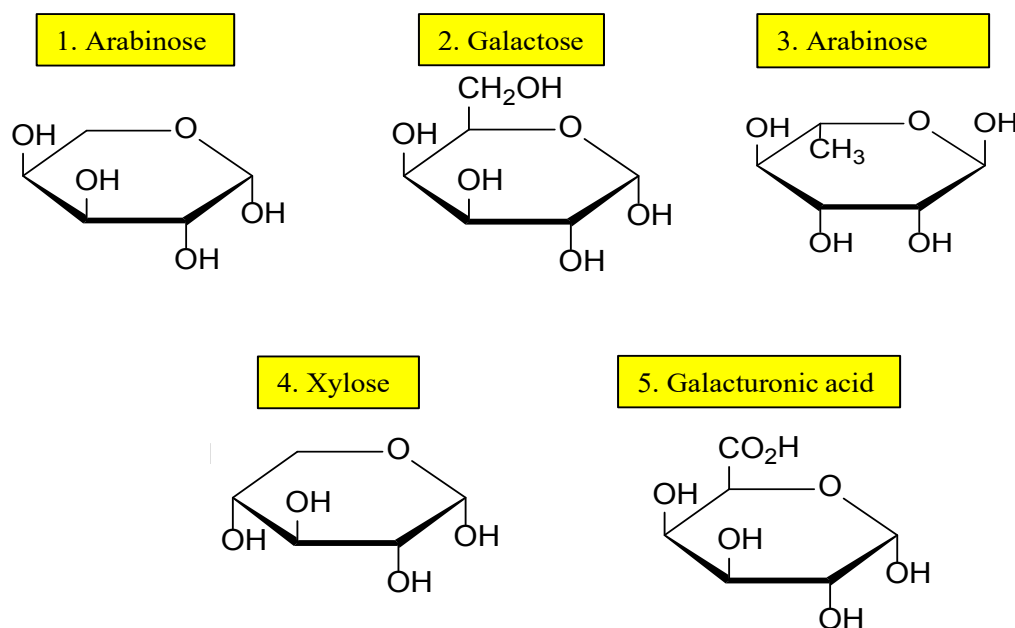
^aMolecular Sciences Institute, University of the Witwatersrand

*Corresponding author: siziwe.gqoba@wits.ac.za

Abstract

Recently, mucilage from the *Opuntia-ficus indicus* (prickly pear) has found traction as an alternative source of biopolymers for the fabrication of bioplastic films.¹ Mucilage is a complex carbohydrate with arabinose (1), galactose (2), rhamnose (3), xylose (4) and galacturonic acid (5) as the most prevalent.^{2,3} This study is aimed at optimizing the extraction of mucilage from *Opuntia ficus-indica* and to evaluate its physicochemical properties for potential application as a biodegradable bioplastic. Initial yields of extracted mucilage were recorded at 2.83% and significantly increased to 11.38% through systematic variation of certain parameters of the extraction method. These parameters included water-to-cladode ratio, temperature, extraction duration, and precipitation solvent-to-plant ratio. Infrared spectroscopy (IR) confirmed the presence of functional groups associated with the mucilage. Meanwhile, X-ray diffraction (XRD) analysis demonstrated that the mucilage was predominantly amorphous, with a low crystallinity index. Scanning electron microscopy (SEM) further supported the amorphous nature, revealing irregular particle shapes and sizes. The carbohydrate content was determined to be 54%, indicating a substantial potential for development as biodegradable bioplastics material.

Keywords: *Opuntia ficus-indica*, mucilage, biodegradable, bioplastics



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A pH-RESPONSIVE COVALENT ORGANIC NETWORK: MORPHOLOGY CHANGE LEADS TO CAPTURE AND REMOVAL OF PHOSPHATE IONS FROM WATER

Gunanka Hazarika ^a, Sribash Das ^b, Niku Moni Das ^b and Debasis Manna ^{*ab}

^aCentre for the Environment, Indian Institute of Technology Guwahati, Assam 781039, India.

^bDepartment of Chemistry, Indian Institute of Technology Guwahati, Assam 781039, India.

*Corresponding author: dmanma@iitg.ac.in

Abstract

Phosphate is one of the essential nutrients for the growth of various organisms. However, it increasingly infiltrates aquatic environments due to human activities, posing environmental risks. Recovering phosphates from wastewater offers a promising solution to mitigate eutrophication and protect dwindling global phosphate reserves. To address this problem, we developed a pH-responsive two-dimensional covalent organic network (2D ag-CON) with multiple interaction sites for anions. Phosphate adsorption resulted in the transition of its surface morphology from spherical to sheet-like structures, providing a distinctive characteristic of ag-CON. The pH-dependent adsorption and desorption properties of the tris-aminoguanidine-based 2D ag-CON enable the selective capture and release of phosphate by adjusting the pH of the solution. The polymer demonstrates high selectivity for phosphate ions, even in the presence of excess competing anions, with a maximum adsorption capacity (Q_{max}) of 719 mg g^{-1} at pH 6 and allows efficient release of captured phosphate ions through pH adjustment ($\square 11.5$). Overall, this study demonstrated the development of a water-insoluble COF capable of efficiently capturing phosphate from wastewater to mitigate the adverse effects of water eutrophication.

Keywords: Phosphate, Eutrophication, ag-CON, pH.

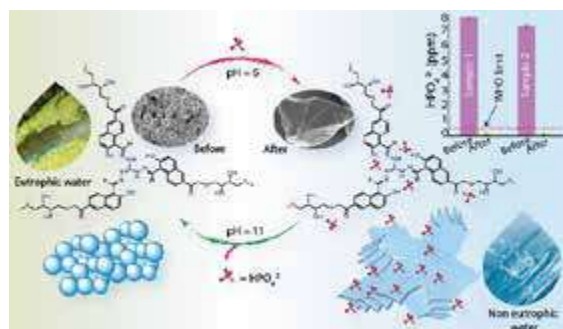


Figure. Graphical abstract of the phosphate removal mechanism from wastewater using tg-CON polymer.

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ANODE ENGINEERING WITH *IN-SITU* COATED UiO-66-NH₂ ON GRAPHITE FOR ENHANCED ANODE PERFORMANCE IN LITHIUM-ION BATTERY

Noor Fazriyana Hamidon^{a,c}, Adam Azizi Abd Azis^a, Hayyiratul Fatimah Mohd Zaid^c, Akmaliah Dzulkurnain^b, Khairulazhar Jumbri^{a,*}

^aDepartment of Fundamental and Applied Science, Center of Research in Ionic Liquids (CORIL), Institute of Sustainable Energy and Resources (ISER), Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia

^bInternational Battery Center, Lot G-4, HIVE 8, Technology Park MRANTI, Bukit Jalil, 57000, Wilayah Persekutuan Kuala Lumpur, Malaysia

^cDepartment of Chemical Engineering, Centre of Innovative Nanostructure and Nanodevices (COINN), Institute of Smart and Sustainable Living (ISSL), Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia

*Corresponding author: khairulazhar.jumbri@utp.edu.my

Abstract

Lithium-ion batteries, which power industries ranging from portable electronics to electric vehicles, have achieved significant commercial success by utilizing lithium ions for intercalation and deintercalation reactions between the anode and cathode electrodes. Traditional graphite anodes face challenges such as structural degradation and reduced cycle life due to solvent molecules embedding and Solid Electrolyte Interphase (SEI) film damage. Coating anode materials can help stabilize the SEI film and improve battery performance. Metal-organic frameworks (MOFs), such as UiO-66-NH₂, are known for their porous structures and customizable properties, making them promising candidates for enhancing battery electrodes. This project aims to synthesize and characterize an in-situ Graphite/UiO-66-NH₂ composite with different UiO-66-NH₂ loadings using the solvothermal method to improve the anode performance of lithium-ion batteries. The composite anodes were prepared with UiO-66-NH₂ loading 5 wt%, 10 wt% and 15 wt% in-situ with Graphite. Their electrochemical performance was evaluated in coin cell batteries over 100 charge-discharge cycles to assess the capabilities and limitations of the anode composite. Additionally, specific capacity and capacity retention were studied to measure the amount of charge the battery can store per unit mass and its ability to maintain storage capacity after multiple cycles. These findings are important for developing efficient, high-energy-output, and cost-effective lithium-ion batteries for long-term applications.

Keywords: Anode, UiO-66-NH₂, Graphite/UiO-66-NH₂, coin-cell

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DEVELOPMENT OF TRANSPARENT SUBSTRATES WITH IMPRINTED PATTERNS FOR STRETCHABLE ELECTRONICS

Min Jae Sung^a, Chul Jong Han^a, Byungwook Yoo^{a,*}

^a Korea Electronics Technology Institute

*Corresponding author: bwwoo@keti.re.kr

Abstract

The development of stretchable transparent electronic circuits and displays integrating thin-film transistors (TFT) requires an organic substrate that balances elasticity, optical transparency, and chemical and thermal durability under fabrication conditions. To meet these requirements, we employed a colorless polyimide capable of withstanding high-temperature processes (~350°C) as the substrate material in the TFT region. In adjacent areas, a highly stretchable organic material was introduced to provide mechanical compliance, forming an island-sea composite substrate structure. Additionally, we present an imprinting-based patterning approach as a cost-effective and scalable alternative to conventional photolithography for structuring the transparent polyimide layer. This method enables precise pattern formation while reducing processing complexity and material waste. The study results highlight the feasibility of this approach for next-generation stretchable transparent electronic systems, providing a route to advanced stretchable transparent applications.

Acknowledgement

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Keywords: transparent substrate, stretchable substrate, colorless polyimide, imprinting

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THERMOELECTRIC PROPERTIES ENHANCEMENT OF Bi_2Te_3 THIN FILM VIA IN DOPING

Angella Th'ng^{a,*}, Nurfarhana Ahmad Musri^a, Puvaneswaran Chelvanathan^a, Mohd Sukor Su'ait^a,
Nadhrhah Md Yatim^b, Assayidatul Laila Nor Hairin^c, Ubaidah Syafiq^{a,*}

^a Solar Energy Research Institute, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

^b Faculty of Science and Technology, Universiti Sains Islam Malaysia (USIM), Bandar Baharu Nilai, 71800, Nilai, Negeri Sembilan, Malaysia

^c Department of Manufacturing and Materials Engineering, Kulliyah of Engineering, International Islamic University Malaysia, Kuala Lumpur, Malaysia

*Corresponding author: ubaidahsyafiq@ukm.edu.my, p153906@siswa.ukm.edu.my

Abstract

Bi_2Te_3 serves as a widely utilized material in sustainable energy conversion because it plays a fundamental role in thermoelectric (TE) applications. However, most studies are done on bulk Bi_2Te_3 since it is easy to fabricate, even though its application is limited due to its rigidity¹. Thin film Bi_2Te_3 presents a more flexible approach, but studies to improve its TE performance are scarce. Compositional control via cationic doping to improve TE performance is necessary to realize new breakthroughs and encourage widespread integration. The introduction of indium (In) dopant is expected to improve TE performance of Bi_2Te_3 thin film by enhancing both structural and electrical properties². Our work examines how different In compositions structurally alter the film, as well as TE power factor (PF), calculated from Seebeck coefficient and electrical resistivity using the equation:

$$ZT = \frac{S^2}{\rho} T$$

where S is the Seebeck coefficient (in $\mu\text{V}/\text{K}$) and ρ is the electrical resistivity (in $\Omega\cdot\text{m}$)³. X-ray diffraction revealed In doping introduces distinct phase compositions within the Bi_2Te_3 thin film. Results showed Bi_2Te_3 as the main phase composition, while Te , In_2Te_3 , In_4Te_3 and Bi_4Te_3 secondary phases were detected as the In concentration increased. S measurements on 0W, 5 W, and 10 W-doped samples showed the decreasing values from -1.26×10^{-4} , -7.87×10^{-5} , to $-7.71 \times 10^{-5} \mu\text{V}/\text{K}$, respectively. Meanwhile, ρ decreased with an increase in doping and 10 W-doped sample achieved the lowest resistivity of $7.18 \times 10^{-5} \Omega\cdot\text{m}$. In-doping essentially creates better electron flow but reduces Seebeck voltage, which ultimately affects TE performance. The calculated PF revealed 0 W-doped sample achieved the highest value of $1.27 \times 10^{-4} \text{ W}/\text{mK}^2$, since it has high S and low enough ρ . Thus, improving TE performance via cationic doping requires optimization to solve the issues of phase segregation and boosting carrier movements⁴. Our results serve as a guide in the development of high-performance thin film TE materials.

Keywords: Bi_2Te_3 thin film, In-doping, thermoelectric, Seebeck coefficient, electrical resistivity.

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YOLK-SHELL $\text{Fe}_3\text{O}_4@\text{P}(\text{DVB-co-MAA})$ MAGNETIC MICROSPHERES LOADED WITH AG NANOPARTICLES AS HIGH-EFFICIENCY CATALYSTS FOR NITROAROMATIC COMPOUND REDUCTION

Yong Jiang^{a,*}, Xinyu Chen^a, Yingrui Nie^a, Wenqian Fan^a, Zhimin Zhao^a, Zhifei Wang^a

^aJiangsu Province Hi-Tech Key Laboratory for Biomedical Research, School of Chemistry and Chemical Engineering, Southeast University

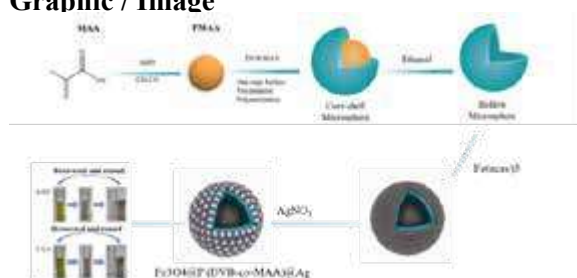
*Corresponding author: yj@seu.edu.cn

Abstract

Yolk-shell magnetic microspheres, characterized by their high specific surface area, unique segregation cavity, and excellent recyclability, hold significant promise for applications in biomedicine, storage, adsorption, and catalysis. While the template-assisted method is frequently employed for the synthesis of yolk-shell microspheres, the complex de-templating step often affects the structure and chemical stability of the microspheres^[1]. This study develops a novel strategy for fabricating magnetic $\text{Fe}_3\text{O}_4@\text{P}(\text{DVB-co-MAA})$ microspheres with yolk-shell architecture. The methodology involves two key steps: (1) constructing hollow poly(divinylbenzene-co-methacrylic acid) [P(DVB-co-MAA)] microspheres via one-step reflux-precipitation polymerization^[2], and (2) uniformly depositing Fe_3O_4 magnetic nanoparticles within the cavity through thermal decomposition of metal-organic precursors in high-boiling-point organic solvents. The resulting microspheres exhibit a distinctive trilayer structure comprising a magnetic core, intermediate void space, and hydrophilic gel shell, demonstrating monodisperse particle size, remarkable colloidal stability, prominent superparamagnetic behavior, and abundant surface carboxyl groups. Precise control over particle dimensions and surface functionality is achievable by modulating monomer ratios and polymerization parameters. Subsequent thermal co-reduction enables in situ growth of silver nanoparticles on the microspheres, yielding magnetic $\text{Fe}_3\text{O}_4@\text{P}(\text{DVB-co-MAA})@\text{Ag}$ composite catalysts. Catalytic evaluations reveal exceptional performance in nitroaromatic reduction (>99% conversion, 95% activity retention after 10 cycles). The ingenious design of this magnetically responsive yolk-shell system endows the multifunctional microspheres with significant potential for applications spanning heterogeneous catalysis, intelligent adsorption, separation, and targeted biomedical delivery.

Keywords: Magnetic material, Yolk-shell structure, Hollow poly(divinylbenzene-methacrylic acid) microspheres, Ag nanoparticles, Catalytic activity.

Graphic / Image



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STRUCTURE-ENGINEERED MICROSPHERES FOR ENHANCED SENSITIVITY IN LUMINESCENT OXYGEN CHANNELING IMMUNOASSAYS

Yingrui Nie ^a, Yong Jiang ^{a*}

^a School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, PR China

* Corresponding author: yj@seu.edu.cn

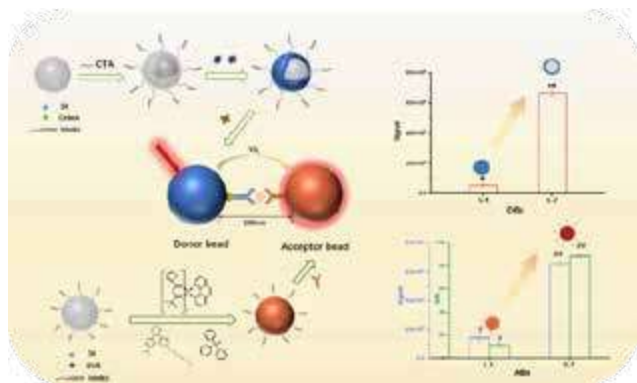
Abstract

Light-activated oxygen channeling immunoassay (LOCI) has gained significant attention in immunoassays due to its advantages of simplicity, sensitivity, and automation. The preparation of donor/acceptor beads (DBs/ABs) is recognized as crucial for detection sensitivity in LOCI systems. In this work, high-performance DBs/ABs were developed to significantly enhance signal intensity and signal-to-noise ratio (S/N) in LOCI detection. The objectives focused on: (1) the fabrication of DBs with high photosensitizer loading capacity and excellent singlet oxygen (¹O₂) transfer efficiency, and (2) the preparation of structurally stable ABs with superior fluorescence properties, with performance evaluation being conducted through SEB antigen detection. The following aspects were systematically investigated:

1. The loading capacity of microspheres with different structures on functional molecules (photosensitizers, Eu complexes, alkenes);
2. The influence of “soft-shell” DBs with varying molecular weights on the signal intensity of immune detection;
3. The enhancement of S/N through preparation of functionalized ABs.

As a result, the “soft-shell” DBs were successfully prepared with a high photosensitizer loading capacity (up to 80.6%), achieving a signal intensity of 6.65×10^5 (13-fold higher than solid microspheres) in LOCI-based SEB detection.^{1,2} Furthermore, the crosslinked ABs were synthesized, exhibiting superior fluorescence properties ($\sim 5 \times 10^5$ a.u.) and an S/N of 88.6 in LOCI immunoassays, representing a 7.9-fold enhancement.³ These advantages validate that the developed microsphere system may be a new strategy for improving the sensitivity of immunodetection applications.

Keywords: LOCI immunoassay, photosensitizer loading, soft-shell microspheres, molecular weight control, immunodetection sensitivity.



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SYNTHESIS, CHARACTERISATION, AND EVALUATION OF PALM OIL-BASED POLYESTERAMIDE FOR CAROTENE SOLID DISPERSION

Nagaloshni Pragalatha^a, Choy Sin Lee^{b,*} and Ki Yan Lam^b

^aCentre of Postgraduate Studies, IMU University, Bukit Jalil, Kuala Lumpur,

^bDepartment of ^bPharmaceutical Chemistry, School of Pharmacy, IMU University, Bukit Jalil, Kuala Lumpur.

*Corresponding author: choysin_lee@imu.edu.my

Abstract

The role of palm oil and its derivatives in lipid-based formulations and drug delivery systems has been widely explored. Palm oil-based polyesteramides (PEA) with multiple functional roles present promising candidates for enhancing poorly water-soluble active ingredients. This work aims to synthesise and characterise palm oil-based PEA and to formulate carotene solid dispersion using the newly synthesised polymer. Diethanolamine and palm stearin were reacted to produce diethanolamide, which was further reacted with a dicarboxylic acid to produce PEA. Characterisation was performed using FTIR, DSC, amine value, and acid value titration methods. Beta-carotene solid dispersions (10–40% w/w) were prepared using PEA as the carrier. FTIR analysis confirmed the presence of functional groups in diethanolamide (DEA), where the hydroxyl (-OH) broad band was observed at 3298 cm⁻¹. The presence of amide functional groups was indicated by the C=O stretching at 1659 cm⁻¹ and N-H bending at 1454 cm⁻¹. At the same time, the decrement of ester C=O stretch at 1730 cm⁻¹ and carboxylic acid C=O stretch at 1730 cm⁻¹ were observed in the diethanolamide samples. In addition, the disappearance of the broad hydroxyl (-OH) peak of diethanolamide (3300–3500 cm⁻¹) and the emergence of ester (-C=O) stretching at 1740 cm⁻¹ while retaining the amide (-C=O-) peak at 1645 cm⁻¹ have confirmed the formation of PEA. DSC thermograms revealed a transformation of the sharp endothermic peak of crystalline carotene (178°C; 157 J/g) into a broad endothermic peak (162°C; 4.7 J/g) in the solid dispersion, confirming the disruption of carotene crystallinity and the formation of an amorphous solid dispersion. The potential of carotene solid dispersion for solid dosage formulation will be further evaluated.

Keywords: Polyesteramide, Palm-Oil, Solid Dispersion.

EFFECT OF MOLECULAR WEIGHT OF POLYETHYLENE GLYCOL AS PLASTICIZER ON IONIC CONDUCTIVITY OF STARCH/LiClO₄ SOLID POLYMER ELECTROLYTE

Nur Azwa Yusrina Ahmad^a, Syuhada Mohd Tahir^{a,*}

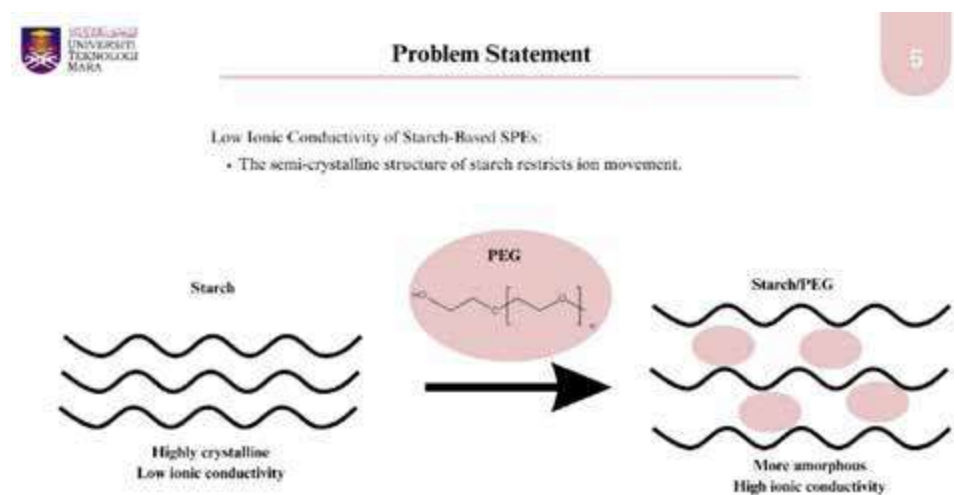
^a*Faculty of Applied Sciences, Universiti Teknologi MARA Pahang, 26400 Bandar Tun Abdul Razak Jengka, Pahang, Malaysia*

^{*}*Corresponding author: syuhadamohdtahir@uitm.edu.my*

Abstract

Petroleum-derived polymers have been widely utilized as hosts in solid polymer electrolytes (SPEs) due to their good ionic conductivity and mechanical stability. However, their dependence on non-renewable resources raises environmental and sustainability concerns. Starch, a biodegradable and renewable biopolymer composed of amylose and amylopectin, presents a promising alternative. Its ionic conductivity originates from oxygen atoms in its polysaccharide structure, which serve as coordination sites for charge carriers. Additionally, starch is abundant, cost-effective, and environmentally friendly, making it a viable candidate for SPE applications. However, its semi-crystalline nature restricts ion mobility, resulting in low ionic conductivity. To overcome this limitation, this study explores the fabrication of starch-based SPEs using potato starch as the polymer host, lithium perchlorate (LiClO₄) as the charge carrier, and polyethylene glycol (PEG) as a plasticizer to enhance ionic transport. Samples were prepared with three PEG variants of different molecular weight; PEG600, PEG1450, and PEG4000 and the effect of PEG molecular weight on the ionic conductivity of starch/LiClO₄ SPEs was evaluated using electrochemical impedance spectroscopy (EIS), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). The SPE with PEG600 exhibited the highest ionic conductivity of 8.59×10^{-4} S/cm, as justified by FTIR results showing a significant OH stretching shift, indicating improved salt-polymer complexation. SEM analysis revealed a smooth surface for starch/LiClO₄/PEG600, facilitating better electrolyte-electrode contact. Conversely, higher molecular weight PEGs (PEG1450 and PEG4000) resulted in rougher surfaces, negatively impacting ionic conductivity. These findings highlight the potential of PEG600 as plasticizer for optimizing starch-based SPEs, paving the way for environmentally sustainable energy storage solutions.

Keywords: starch, biopolymer, solid polymer electrolyte, ionic conductivity



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ELIMINATING TRIBOELECTRIC EFFECTS IN FLEXIBLE DEVICES: A STRATEGIC APPROACH FOR ANTISTATIC COATINGS AND TRIBO-LESS PIEZOELECTRIC RESPONSE

Anshika Passi¹, Tridib Kr. sinha¹

¹University of petroleum and energy studies - Dehradun (India)

Corresponding author: anshika@ddn.upes.ac.in

Abstract

Flexible electronic devices often require polymeric protective layers to maintain their flexibility and safety. However, most polymers are inherently triboelectric, and their triboelectric behavior is highly sensitive to environmental conditions, particularly humidity. Under low or no humidity, triboelectric systems exhibit significantly higher output compared to high-humidity conditions. For instance, the familiar experience of an electric shock from a metal door handle during winter (caused by the discharge of triboelectric charge) is rarely encountered in the rainy season. The similar phenomenon has been observed with various polymer (mainly PVDF and its copolymer)-based flexible piezoelectric devices (in-house developed or commercially available coated with different other polymers e.g., PET, PDMS, etc.) producing major differences in the responses taken under different humidity, higher at lower humidity, signifying presence of triboelectricity along with the piezoelectricity. Piezoelectricity being intrinsic in nature, the device is thus expected to produce a stable response irrespective of place, time, or any environmental conditions. This kind of anomaly may observe with other flexible devices too. In case of PVDF-based bare piezoelectric film, PVDF being highly tribo-negative material, it may also produce the similar synergistic influence while investigating its piezoelectric response. Following the effective washing out charges by polar solvents like water, it has been observed that the generation of triboelectric charges is negligible in high humidity conditions, whereas piezoelectricity remains largely unaffected. This finding underscores the need for strategies to suppress triboelectric effects while preserving the intrinsic piezoelectric response, irrespective of environmental variations. The study aims to develop measurement strategies, antistatic coating materials (via formulating composites of tribo-negative polymers with tribopositive filler materials which are mostly bio-inspired), self-polarized PVDF composites with different bio fillers to address these aforementioned challenges. These innovations will not only contribute to the development of highly reliable piezoelectric systems for diverse applications, including wearable energy harvesters, tactile sensors, and artificial skin, but also paving the way for broader applications in polymer-based flexible sensors and energy harvester applications.

Keywords: Piezoelectricity, triboelectricity, energy harvesting, anti-static coating, bio inspired, polymer composite

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INTERACTIONS AT MATERIAL-BIOFILM INTERFACES: PRELIMINARY SYNCHROTRON-BASED STUDIES FOR NEXT-GENERATION LIVING COATING SYSTEMS

Wojciech Pajerski ^{a,b,*}, Katarzyna M. Sowa^c, Pawel Korecki ^{c,d}, Pawel Wrobel^e,
Tomasz Kolodziej^c, Faksawat Poohphajai^a, Anna Sandak^{a,b,f}

^a InnoRenew CoE, Livade 6a Izola, Slovenia

^b Andrej Marušič Institute, University of Primorska, Slovenia

^c SOLARIS National Synchrotron Radiation Centre, Poland

^d Institute of Physics, Jagiellonian University, Poland

^e Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland.

^f Faculty of Mathematics, Natural Sciences and Information Technologies, University of Primorska, Slovenia

* Corresponding author: wojciech.pajerski@innorenew.eu

Abstract

Developing new sustainable materials often involves integrating biological systems into conventional material structures. Engineered Living Materials (ELMs), incorporating microorganisms represent a promising strategy for designing adaptive, self-healing, and environmentally responsive surface technologies. A critical aspect of this approach involves understanding how biofilms interact with material interfaces, especially in architectural contexts.

This study explores the potential of synchrotron-based X-ray microtomography (μ CT) for investigating material-biofilm interfaces. Using *Aureobasidium pullulans* biofilms grown on wood samples (*Pinus sylvestris* L.), we conducted preliminary high-resolution 3D imaging at the POLYX beamline of the SOLARIS Synchrotron facility. Initial scans demonstrated the feasibility of capturing high-resolution 3D images, providing insights into hyphal network formation, substrate penetration, and biofilm integrity without compromising the natural state of the samples.

This advanced imaging technique provides a deeper understanding of fungal interactions with architectural materials, highlighting their interface and revealing their impact on structural integrity. Such insights are particularly relevant for the development of sustainable coating systems. This foundational work establishes a basis for future research on biofilm interactions across various materials and surfaces.

By focusing on material–biofilm interactions, this study supports the integration of microbial systems into sustainable coating design. The results offer valuable insight for developing next-generation, adaptive, self-healing surfaces that contribute to SDG13 (Climate Action) and promote environmentally responsible material innovation.

Keywords: biointerfaces, material–biofilm interactions, synchrotron imaging, Engineered Living Materials, sustainability

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GREEN STRATEGIES FOR NEXT-GENERATION COATING SYSTEMS: MICROBIAL APPROACHES AT MATERIAL INTERFACES

Wojciech Pajerski ^{a,b,*}, Anja Černoša ^{a,b}, Ana Gubenšek ^{a,b}, Anna Sandak ^{a,b,c}

^a *InnoRenew CoE, Livade 6a Izola, Slovenia*

^b *Andrej Marušič Institute, University of Primorska, Slovenia*

^c *Faculty of Mathematics, Natural Sciences and Information Technologies,
University of Primorska, Slovenia*

* *Corresponding author wojciech.pajerski@innorenew.eu*

Abstract

Advancing sustainable coating systems requires innovative approaches that combine functionality, environmental compatibility, and material durability. This work presents a bio-based approach aligned with green chemistry principles for next-generation surface technologies, integrating microbial systems into materials development. Designed as living coatings, these systems offer potential for carbon sequestration, pollutant capture, oxygen production, and durability with self-healing properties.

The coating functionality is achieved through the selection and spatial organization of metabolically active microorganisms, tailored to support material compatibility and enhance surface performance. Computational tools, including metabolic modeling and machine learning, guide the formulation of stable and responsive microbial assemblies suited to diverse substrates.

The REMEDY project provides the research framework for advancing this approach, combining microbiology, materials chemistry, and sustainable design. Emphasis is placed on compatibility with porous and non-porous substrates, the development of nutrient-efficient formulations, and the potential for circular use cycles. These living coatings contribute to the evolution of Engineered Living Materials (ELMs) and represent a shift toward biologically enhanced materials with built-in adaptability.

This work aligns with the principles of green chemistry and the Safe and Sustainable by Design (SSbD) framework. It also directly contributes to the United Nations Sustainable Development Goals (SDGs), particularly: 3, 7, 9, 11, 12, 13, and 15, by proposing coatings that reduce chemical inputs, extend material life, and enable intelligent environmental response.

Keywords: sustainable coatings, biointerfaces, surface functionality, SDG, engineered living materials

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IMPROVED POLAR VOC DETECTION WITH AN INORGANIC-ORGANIC HYBRID CHEMIRESENSITIVE SENSOR: EXAMINING SENSITIVITY, SELECTIVITY, AND ENVIRONMENTAL EFFECTS

Shreshth Dobriyal^a, Tridib Kumar Sinha^{a*}

^a*Department of Chemistry, Applied Science Cluster, School of Engineering (SoE),
University of Petroleum and Energy Studies (UPES), Bidholi, Dehradun, Uttarakhand 248007, India*

**Corresponding author: Tridib.sinha@ddn.upes.ac.in*

Abstract

Detection and quantification of volatile organic compounds (VOCs) are critical for understanding environmental pollution and its direct impact on human health. These carbon-based compounds, characterized by their low boiling points, are emitted from different sources. Due to their volatility and functional diversity, VOCs are often present as complex mixtures, making their real-time monitoring both important and technically challenging. Traditional sensing technologies often fall short in selectivity, sensitivity, and adaptability across environmental conditions. Metal oxide sensors (MOS), while effective at elevated temperatures, frequently alter the chemical signatures of VOCs. On the other hand, organic semiconductor-based sensors, suitable for ambient operation, suffer from slow response-recovery cycles and limited reuse. These limitations necessitate advanced sensing platforms that can function accurately, repeatedly, and cost-effectively across different conditions. This study proposes a hybrid chemiresistive sensor integrating polyaniline (PANI), reduced graphene oxide (RGO), and zinc oxide (ZnO), synthesized in-situ. The sensor, referred to as PRZ, is designed to detect polar VOCs such as methanol, ethanol, acetone, isopropanol, chloroform, ethyl ether, DMSO, and acetonitrile. The interaction between the VOC molecules and the sensor's active surface leads to distinct changes in electrical resistance, allowing for accurate quantification at both low and room temperatures. Sensor performance is influenced by molecular parameters such as weight, boiling point, geometry, ambient humidity, and temperature. These variables impact the adsorption behavior and electron transfer at the sensing interface. Principal component analysis (PCA) is employed to enhance differentiation and classification of VOCs, even in complex environments. The PRZ sensor demonstrates high sensitivity, selectivity, repeatability, and fast response and recovery times. Its simple fabrication, cost-efficiency, and scalability make it suitable for applications in environmental surveillance, non-invasive diagnostics, and industrial quality control. The integration of nanomaterials in this system presents a promising path toward robust, real-world VOC monitoring solutions.

Keywords: Volatile Organic Compounds (VOCs), Chemiresistive Sensor, Polyaniline-Graphene-Zinc Oxide (PRZ), Real-Time Gas Sensing

SELECTIVE ION-TRANSPORTING POLYMERIC LAYERS FOR ADVANCED ZINC ION BATTERIES

Yanghyun Cho^a, Jongha Hwang^a, Dong Ok Shin^{b,c*}, Minsu Gu^{d*}, and Woo-Jin Song^{a,e,f*},

^aDepartment of Chemical Engineering and Applied Chemistry, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^bMaterials and Components Research Division, Electronics and Telecommunications Research Institute (ETRI), 218 Gajeongno, Yuseong-gu, Daejeon 34129, Republic of Korea.

^cDepartment of Semiconductor and Advanced Device Engineering, University of Science and Technology (UST), 217 Gajeongno, Yuseong-gu, Daejeon 34113, Republic of Korea.

^dDepartment of Chemical Engineering (BK21 FOUR), Dong-A University, 37, Nakdong-daero 550 beon-gil, Saha-gu, Busan 49315, Republic of Korea.

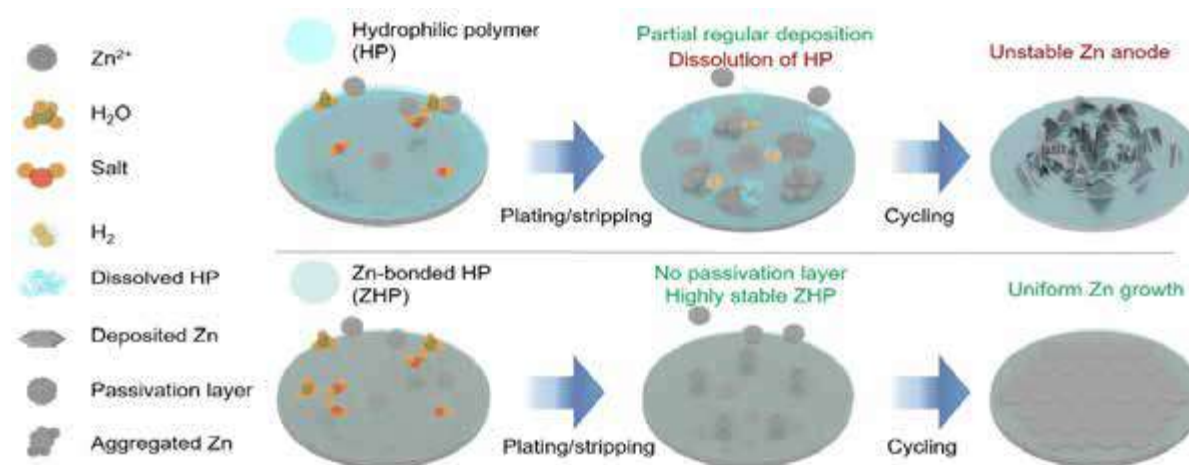
^eDepartment of Material Science Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^fDepartment of Organic Materials Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

*Corresponding author: doshin@etri.re.kr (D. O. Shin), sbgms@dau.ac.kr (M. Gu), and wjsong@cnu.ac.kr (W. -J. Song)

Abstract

Aqueous Zinc-ion batteries (AZIBs) are promising energy-storage devices; however, dendrite growth and undesirable reactions impede their advancement.¹ To overcome these issues, we designed a Zn-bonded ion-selective layer using poly (acrylic acid) (PAA) modified by O₂ plasma treatment. This layer improves electrolyte wettability adhesion and suppresses undesired reactions by capturing anionic salts. The Zn@ZHP symmetric cell shows a remarkable lifespan of 2,200 hours at 10 mA cm⁻², greatly surpassing the 250 hours of bare Zn. In full cells (Zn@ZHP||Zn_{0.25}V₂O₅), 95% capacity is retained after 500 cycles at 1 A g⁻¹, compared to 75.4% for the control. Additionally, pouch-type cells demonstrate stable cycling for over 300 cycles at 5 A g⁻¹. These results highlight the effectiveness of the ZHP interface in mitigating dendrites and stabilizing the Zn anode, offering a promising approach for improving the performance and durability of AZIBs.²



Keywords: poly (acrylic acid), zinc anode, oxygen plasma treatment, selective ion transport layer, aqueous Zinc-ion batteries (AZIBs)

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INTERFACE MODIFICATION OF POLYMER NANOCOMPOSITE FILM FOR PRINTABLE NANO-FLOATING GATE MEMORY

Kailin Tang^a, Renhua Deng^{a*}, Jintao Zhu^a

^aHuazhong University of Science and Technology, Wuhan 430074, China

*Email: rhdeng@hust.edu.cn

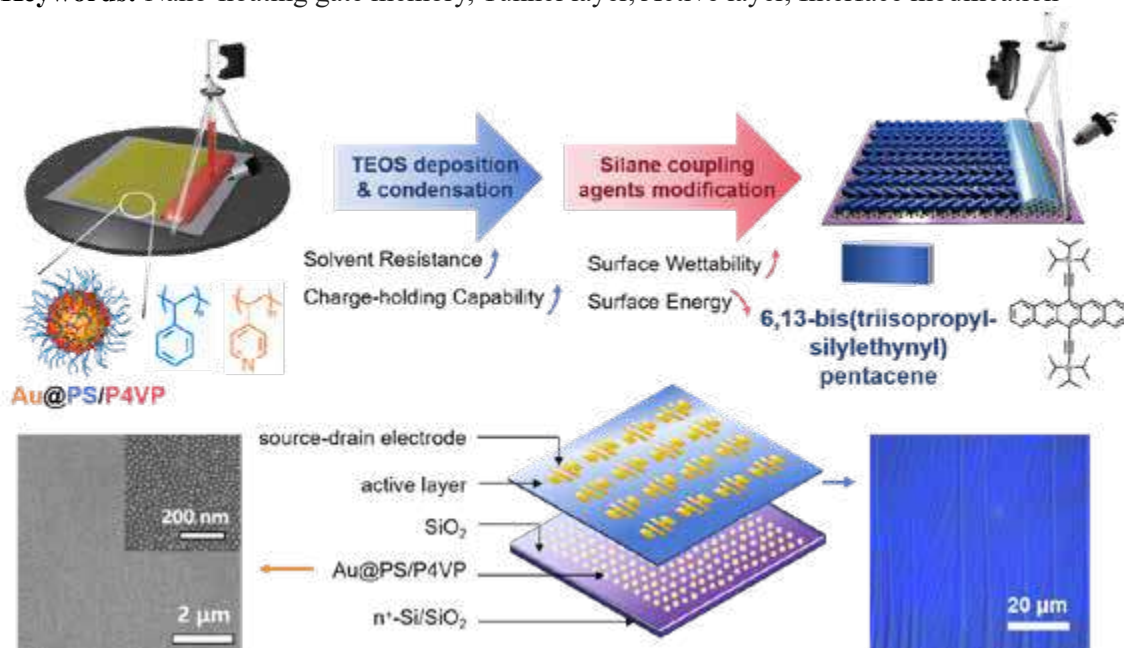
Abstract

Nano-floating gate memory (NFGM) is a leading candidate for next-generation non-volatile memory. This study focuses on enhancing the performance and stability of NFGM by modifying the tunnel layer/active layer interface and optimizing the active layer structure. This discussion will focus on the following key points with the goal of performance enhancement:

1. Preparation of binary polymer-grafted gold nanoparticle (Au@PS/ P4VP) monolayers as nano-floating gate/tunneling layer (NFG/TL) by fiber printing
2. In situ growth of SiO₂ on NFG/TL surfaces
3. Preparation of highly oriented active layers by fiber printing

The key findings include the effective improvement of the solvent-resistance of NFG/TL layer and the optimization of the orientation of active layer, leading to enhanced memory window (40 V) and retention performance. These advancements provide new insights into the development of high-performance NFGM devices.

Keywords: Nano-floating gate memory, Tunnel layer, Active layer, Interface modification



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INITIATOR-FREE CROSSLINKING PROCESS WITHOUT ORGANIC SOLVENT FOR LITHIUM METAL BATTERIES BASED ON POLYMER ELECTROLYTE

Sanghyun Park^a, Chi Keung Song^b, Mincheol Jung^b, Seong Min Jeon^a, Changhee Chae^a,
Woo-Jin Song^{b, c*}, Kyung Jin Lee^{a*}

^aDepartment of Chemical Engineering and Applied Chemistry, College of Engineering, Chungnam National University, W3-453, 99, Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea

^bDepartment of Chemical Engineering and Applied Chemistry, College of Engineering, Chungnam National University, W3-484, 99, Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea

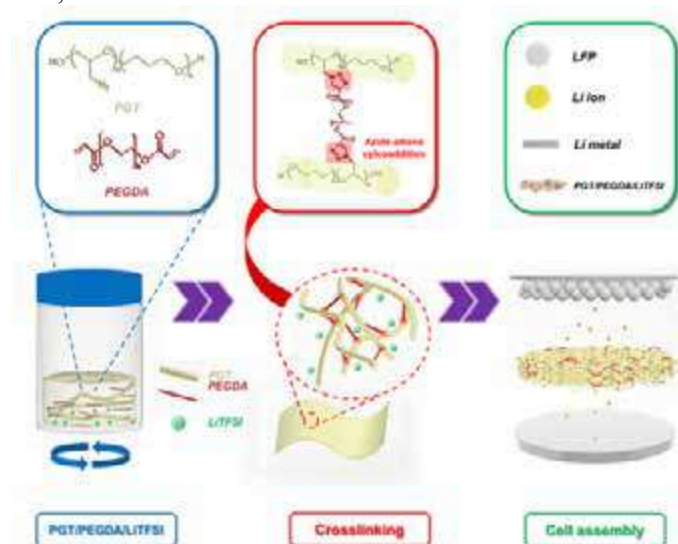
^cDepartment of Materials Science and Engineering, College of Engineering, Chungnam National University, Yuseong -gu, Daejeon 34134, Republic of Korea

*Corresponding author: wjsong@cnu.ac.kr (W. -J. Song), kjlee@cnu.ac.kr (K.J. Lee)

Abstract

Polymer-based electrolytes are promising candidate as a possible replacement for liquid electrolytes (LE) with safety issues such as leakage and flammability in next-generation lithium batteries. Various polymeric materials (PAN, PVDF, PEO) have been proposed as materials for polymer electrolytes, among which PEO has been identified as a promising electrolyte material due to its high ionic conductivity and flexible polymer chain structure based on the segmental motion of Li⁺ ions. In this study, Poly(GAP-co-THF) diol (PGT), featuring a PEO-like backbone and azide side groups, was prepared and thermally cross-linked with PEGDA and LiTFSI via azide-alkene cycloaddition without initiators or solvents. Thickness controllable thin film of polymer electrolyte was obtained after thermal crosslinking process, resulting in outstanding advantages with respect to stacking of batteries. To check out electrochemical stabilities and cell performances of these polymer electrolytes, cyclic voltammetry (CV), linear symmetric voltammetry (LSV), LiFePO₄(LFP) || Li cell, and Li symmetric cell test were accomplished

Keywords: thermal crosslinking, azide-alkene cycloaddition, polymer electrolytes, lithium metal batteries, initiator-free, solvent-free



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PLLA-BASED MODIFIED FOOD PACKING MATERIALS

Jie Cao^a, Jiahui Du^a, Xueyan Yun^a, Tungalag Dong^{a,*}

^a College of Food Science and Engineering, Inner Mongolia Agricultural University

*Corresponding author: dongtlg@163.com

Abstract

With the increase of white pollution, poly (L-lactic acid) (PLLA) is regarded as an ideal candidate to replace traditional plastics. However, PLLA suffers from shortcomings such as average barrier properties and poor blow moulding performance, which limit its wide application in food packaging. The focus of this study is on the development of PLLA-based packaging materials. In this study, we synthesised the terpolymer poly(L-lactic acid-co-butylene glycol ester) (PLBI) by introducing poly(itaconic acid-co-butylene glycol) (PBI) into the PLLA backbone via melt polycondensation; and composite films with high barrier properties and high toughness were prepared by UV cross-linking. At the same time, fresh air-conditioned packaging with excellent flexibility and selective permeability was prepared by using a blend to modify the blow moulding properties of PLLA. In this context, several points deserve further discussion.

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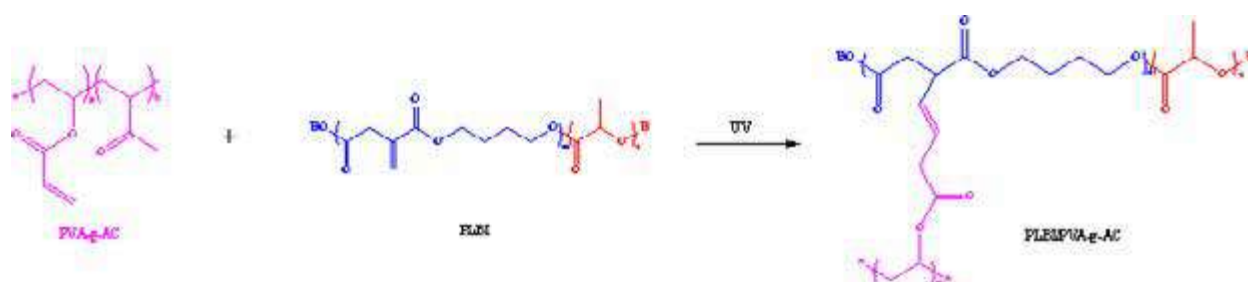
1. Development of PLBI films with high toughness and high barrier properties ¹.
2. Preparation of PLBI/PVA-g-AC high barrier, high tenacity food packaging film. ².
3. Preparation of PLLA/PBAT/P(LA-BI) high toughness, high selective permeability blown films.

As a result, successful development of PLLA-based high tenacity, high barrier or high permeability films.

Keywords: polylactic acid-based composite film, high barrier packaging, High selective permeability packaging, modified

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DYNAMIC CROSSLINKED SELF-HEALING BINDER FOR HIGH-PERFORMANCE SILICON ANODES

Minju Song^a, Woo-Jin Song^{a,b,c*}

^aDepartment of Chemical Engineering and Applied Chemistry, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^bDepartment of Material Science Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

^cDepartment of Organic Materials Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon 34134, Republic of Korea.

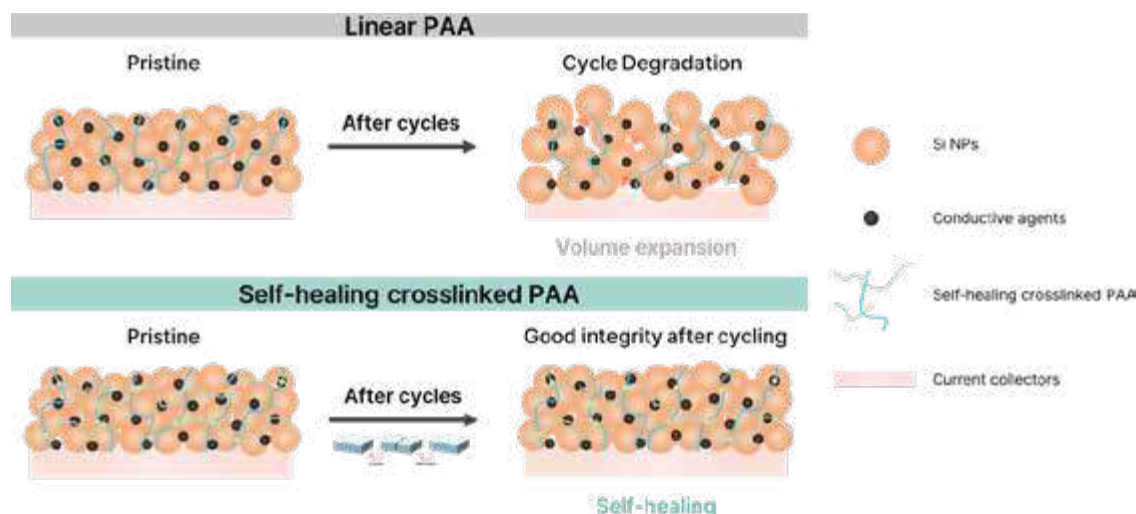
*Corresponding author: wjsong@cnu.ac.kr (W. -J. Song)

Abstract

Silicon (Si) is considered a highly promising anode material for next-generation lithium-ion batteries (LIBs) due to its exceptionally high theoretical specific capacity of 4,200 mAh g⁻¹. However, the substantial volume expansion (>300%) during lithiation and delithiation leads to severe structural pulverization and rapid capacity degradation, posing significant challenges for practical implementation. To overcome these limitations, a novel crosslinked self-healing PAA(c-SHPAA) binder was developed by incorporating dynamic bonding functionalities into a poly (acrylic acid) (PAA) matrix. This binder system leverages reversible dynamic bonds to autonomously repair cracks generated during cycling, while the crosslinked network provides enhanced mechanical robustness to accommodate the large volume changes of silicon particles. When applied to Si anodes, the c-SHPAA binder exhibited a high initial coulombic efficiency of 91% and a reversible capacity of 3,866 mAh g⁻¹, while maintaining over 83% capacity retention after 100 cycles at a current density of 0.5C. These results confirm that the c-SHPAA binder effectively mitigates the volume fluctuation of silicon anodes and significantly improves their long-term cycling stability. This work highlights a promising binder design strategy for advancing high-capacity and durable anodes in next-generation lithium-ion batteries.

Keywords: poly (acrylic acid), Silicon Anode, Self-Healing Polymer Binder, Lithium-ion Batteries (LIBs), dynamic crosslinks

Graphic / Image



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SMART POLYMERS IN DRUG DELIVERY: ADVANCING PRECISION MEDICINE FOR SAFER AND TARGETED THERAPEUTICS

Zainab Ngaini and Vannessa Lawai

Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak

Corresponding author: nzainab@unimas.my

Abstract

Aspirin is a widely used non-steroidal anti-inflammatory drug for analgesic and cardio-protection. However, it is often limited by gastrointestinal side effects such as mucosal irritation and bleeding.

Molecularly imprinted polymers (MIPs) offer a promising platform for controlled and targeted drug delivery due to their highly specific recognition sites tailored to the drug molecule. This study presents a rapid microwave (MW)-assisted synthesis of aspirin-imprinted MIPs using methacrylic acid and divinylbenzene and optimized via Central Composite Design. MW synthesis significantly produced smaller spherical particles polymers (500 nm–1.45 μ m) in 8 minutes at 110°C with higher yields (0.5–1.2 g) and superior aspirin rebinding capacity (7.15 ± 0.02 mg/g) compared to conventional heating (660 nm–3.65 μ m, 0.5–1.15 g, 3.00 ± 0.31 mg/g, 6 hours), respectively. *In vitro* release studies demonstrated excellent diffusion-controlled aspirin release consistent with Higuchi kinetics models with enhanced release at intestinal pH (7.4) relative to gastric pH (2.2), indicating suitability for targeted intestinal delivery. This study demonstrates fast, efficient and tunable approach for developing intelligent drug carriers that improve therapeutic efficacy while minimizing systemic toxicity and gastrointestinal side effects in drug administration strategies.

HIGH-PERFORMANCE POLYMER-BASED LUMINESCENT SOLAR CONCENTRATORS ENABLED BY MDMO-PPV: EFFICIENCY, STABILITY, AND SCALABILITY

Betul Canimkurbey^{a,b*}, Furkan Isik^{b,c}

^a Department of Physics, Faculty of Polath Science and Art, Ankara Hacı Bayram Veli University, Ankara 06900, Turkey.

^b Department of Electrical and Electronics Engineering, Department of Physics, UNAM – Institute of Materials Science and Nanotechnology and The National Nanotechnology Research Center, Bilkent University, Ankara 06800, Turkey.

^c Institute of Accelerator Technologies, Ankara University, Ankara, Turkey

*Corresponding author: betul.canimkurbey@hbv.edu.tr

Abstract

Luminescent solar concentrators (LSCs) are emerging scalable solutions for enhancing photovoltaic efficiency, particularly in building-integrated and portable energy systems. Conjugated polymers, owing to their tunable optical properties, ease of processing, and mechanical flexibility, present a promising class of luminophores. Poly[2-methoxy-5-(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene] (MDMO-PPV) exhibits a broad absorption spectrum and high photoluminescence quantum yield, positioning it as a strong candidate to address the limitations of previously studied polymer-based LSCs. Despite its advantageous optoelectronic characteristics, the use of MDMO-PPV in LSCs remains largely underexplored. This study focuses on the fabrication and optical characterization of MDMO-PPV-based LSCs, evaluating their optical efficiency and benchmarking their performance against established polymeric systems. Key challenges in LSC optimization, such as reabsorption losses and limited Stokes shifts, are addressed through potential molecular engineering approaches and photonic design strategies. The absorption spectrum displays a broad band spanning approximately 400–550 nm, with a pronounced peak centered around 470 nm, corresponding to π - π^* electronic transitions along the conjugated polymer backbone, which facilitates efficient harvesting of a significant portion of the visible solar spectrum. The dominant emission peak at ~590 nm yields a substantial Stokes shift of ~120 nm, which results in reduced reabsorption, one of the primary loss mechanisms in waveguide-based devices. The optical performance of the MDMO-PPV-based LSCs devices was evaluated through power conversion efficiency (η_{power}) measurements using an integrating sphere setup. The highest optical power conversion efficiency of LSC devices were recorded as 2.7%, which stands out among polymer based LSCs. The results validate MDMO-PPV as a high-performing polymeric luminophore for LSCs, offering excellent spectral properties and stability. This work supports the integration of MDMO-PPV into low-cost, scalable LSCs and opens new avenues for efficient solar energy harvesting via polymer-based architectures.

Keywords: Conjugated polymers, MDMO-PPV, luminance solar concentrator, reabsorbtion

BIOWASTE-DERIVED COMPOSITE MEMBRANES FOR OIL/WATER SEPARATION

Nurul Amni Abdullah^{a, c}, Azizah Baharum^a, and Rizafizah Othaman^{a*}

^a Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600, Selangor, Malaysia;

^b Faculty of Applied Sciences, Universiti Teknologi MARA Perak Branch, Tapah Campus, 35400 Tapah Road, Malaysia.

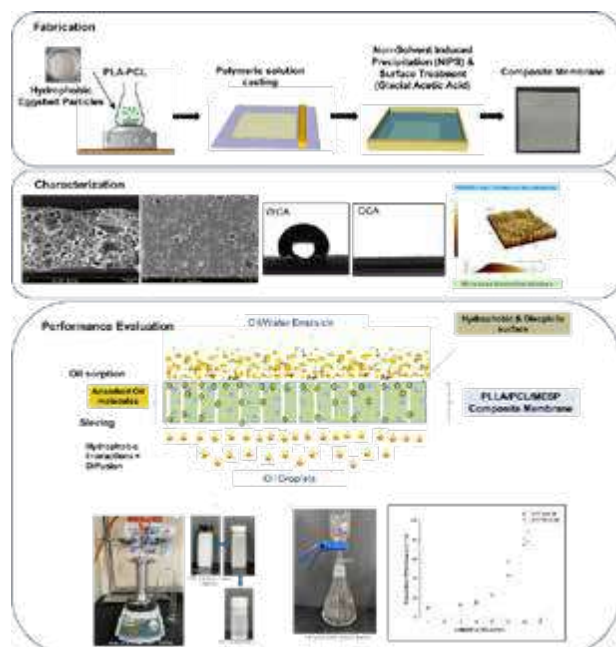
*Corresponding author: rizafizah@ukm.edu.my

Abstract

Oil-in-water (O/W) emulsions in domestic and industrial effluents pose a multifaceted challenge due to their stability, low droplet size, and resistance to traditional treatment methods. In this study, composite microfiltration membranes were developed to efficiently separate oil droplets from O/W emulsions. Chicken eggshell particles were chemically modified via esterification and directly incorporated into a poly(L-lactic acid)/polycaprolactone (PLLA/PCL) matrix, forming a homogeneous, porous, and asymmetric membrane with a micro/nano-hierarchical structure that enhances surface hydrophobicity. The membranes were fabricated using a combination of plate casting, non-solvent-induced phase separation (NIPS), acid treatment, and ambient drying. A comprehensive characterization of the membranes was conducted, including chemical structure, morphology, crystallinity, mechanical strength, and surface wettability. The filtration performance was evaluated using a surfactant-stabilized O/W emulsion. This work demonstrates a sustainable approach to valorizing biowaste eggshells while providing a high-performance membrane for efficient oil/water separation.

Keywords: esterification, polymer composite, thin membrane, hydrophobic, oil/water separation

Graphic / Image:



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INHIBITIVE EFFECT OF TRIDENTATE HYDRAZONE LIGANDS TOWARDS CORROSION OF MILD STEEL IN 3.5% NaCl SOLUTION SATURATED WITH CO₂

Balqis Auni Badrul Hisyam^a, Zainiharyati Mohd Zain^{a,b}, NurulFazlina Edayah Rasol^{a,c}, Noor Asnida Asli^c, Amalina Mohd Tajuddin^{a,c*}

^a Faculty of Applied Sciences, Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia.

^b Electrochemical Material and Sensor (EMaS), Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia.

^c Atta-ur-Rahman Institute for Natural Product Discovery (AuRIns), UiTM Puncak Alam, 42300, Bandar Puncak Alam, Selangor, Malaysia.

^d Centre of Functional Materials and Nanotechnology (FMN), NANO-SciTech Lab (NST), Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia.

*Corresponding author: amalina9487@uitm.edu.my

Abstract

Continuous research and demand for affordable and eco-friendly anti-corrosion agents against CO₂ corrosion in the petroleum industry have driven the development of sustainable tridentate hydrazone ligands to effectively protect the mild steel from CO₂ attack. Hydrazone ligands (AL01-AL04) derived from benzohydrazide and 2-hydroxybenzohydrazide were successfully synthesized and characterized using melting point, FTIR, NMR, elemental analysis, UV-Vis, and mass spectroscopy. The formation of hydrazone ligands was confirmed by the appearance of the $\nu(\text{C}=\text{N})$ peak in the range 1605 to 1648 cm⁻¹. The significant peak of azomethine protons (HC=N) for AL01-AL04 appeared at 8.82, 8.41 8.58, 8.76 ppm, respectively, while the peak of phenolic protons (O-H) for AL01 and AL03 was found at 12.28 and 11.56 ppm respectively. Single crystal X-ray diffraction revealed that both AL03 and AL04 crystallized as orthorhombic systems in the Pbc_a and Pbc_n space groups, respectively. The corrosion inhibition performance of AL01-AL04 inhibitors for mild steel in CO₂-saturated 3.5% NaCl solution was examined using polarization and impedance spectroscopy. Results demonstrate AL01 as the most effective inhibitor as the polarization resistance (R_{ct}) values rose from 393.76 to 941.24 Ω cm² with an increase in AL01 concentration. AL01 exhibited the highest corrosion inhibition efficiency, 84.30% at 500 ppm, with the lowest I_{corr} value of 13.132 $\mu\text{A}/\text{cm}^2$ which indicates a reduction in the corrosion rate. The surface morphology (FESEM-EDX and AFM) has confirmed the development of a protective film on the mild steel surface. Theoretical data from DFT calculations further corroborate the experimental findings regarding the adsorption and inhibition capabilities of the ligands. The presence of heteroatoms, pyridine, and aromatic rings facilitates the adsorption of hydrazone ligands onto the mild steel surface for protection against corrosion. XPS analysis has identified the presence of C=C (283.74 eV), C=O (288.2 eV) and C-N (398.32 eV) attributed to the adsorption of AL01 on the mild steel surface^{1,2}.

Keywords: benzohydrazide tridentate hydrazones, 3.5% NaCl, CO₂, EIS, XPS.

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BIOWASTE-DERIVED COMPOSITE MEMBRANES FOR OIL/WATER SEPARATION

Nurul Amni Abdullah^{a,c}, Azizah Baharum^a, and Rizafizah Othaman^{a*}

^a Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600, Selangor, Malaysia;

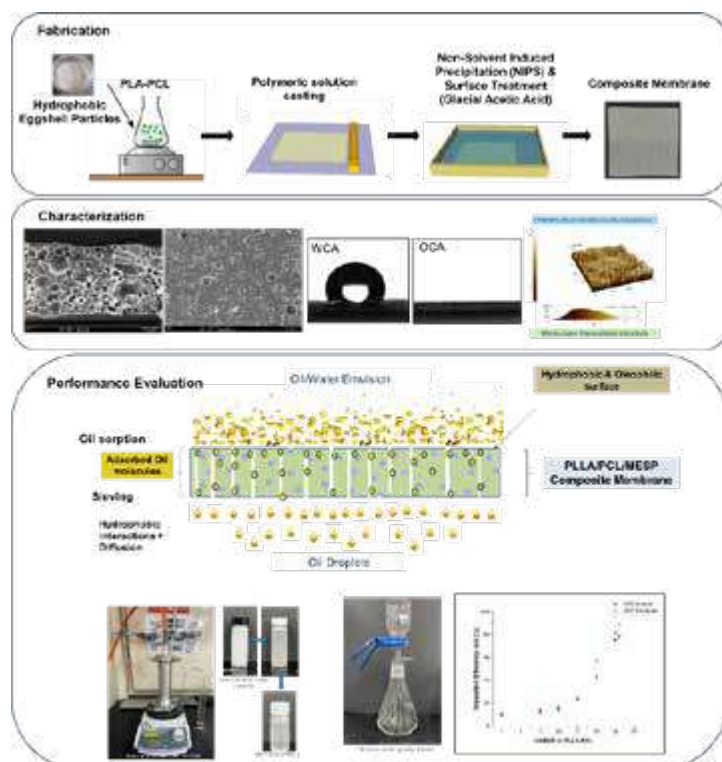
^b Faculty of Applied Sciences, Universiti Teknologi MARA Perak Branch, Tapah Campus, 35400 Tapah Road, Malaysia.

*Corresponding author: rizafizah@ukm.edu.my

Abstract

Oil-in-water (O/W) emulsions in domestic and industrial effluents pose a multifaceted challenge due to their stability, low droplet size, and resistance to traditional treatment methods. In this study, composite microfiltration membranes were developed to efficiently separate oil droplets from O/W emulsions. Chicken eggshell particles were chemically modified via esterification and directly incorporated into a poly(L-lactic acid)/polycaprolactone (PLLA/PCL) matrix, forming a homogeneous, porous, and asymmetric membrane with a micro/nano-hierarchical structure that enhances surface hydrophobicity. The membranes were fabricated using a combination of plate casting, non-solvent-induced phase separation (NIPS), acid treatment, and ambient drying. A comprehensive characterization of the membranes was conducted, including chemical structure, morphology, crystallinity, mechanical strength, and surface wettability. The filtration performance was evaluated using a surfactant-stabilized O/W emulsion. This work demonstrates a sustainable approach to valorizing biowaste eggshells while providing a high-performance membrane for efficient oil/water separation.

Keywords: esterification, polymer composite, thin membrane, hydrophobic, oil/water separation



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QUALITY ASSURANCE IN LATEX PRODUCTS MANUFACTURING: WHAT IS NEEDED FOR FURTHER IMPROVEMENT

Eng Aik Hwee

^aK&W Training & Consulting

**Corresponding author: engaikhwee@gmail.com*

Abstract

Manufacturing of latex products such as rubber gloves and condoms requires strong technical knowledge as well as hands-on experience for consistent product quality. Unlike dry rubber, maintaining latex stability and homogeneity, and managing bubbles in coagulant and latex during the production process are some of the typical challenging tasks. In addition, the intra-particle and inter-particle crosslinks, prevulcanisation and post-vulcanisation, and different sulphidic crosslinks could significantly impact the performance of the products such as heat and solvent resistance, as well as tensile properties. Better controls on the quality of incoming raw materials, latex compounding and processing, are expected to help reduce product defects, leading to consistent product quality. On the other hand, insufficient control will cause inconsistent product quality and make troubleshooting difficult. Insufficient control could be the control methods are unavailable, too expensive, too complicated, or unknown to the manufacturers. This paper examines some of the more important parameters that significantly affect the quality of latex products and the corresponding monitoring methods. For important but unavailable or tedious methods, it is hoped that some researchers could help to develop or simplify them for the industry to adopt.

Keywords: Latex products, processing, quality assurance, monitoring methods

INNOVATING NATURAL LATEX: FROM SCIENTIFIC FOUNDATIONS TO SUSTAINABLE INDUSTRIAL APPLICATIONS

Jitladda Sakdapipanich^{1*}

*^aRubber Research Group, Department of Chemistry, Faculty of Science,
Mahidol University, Nakhon Pathom 73170, Thailand.*

**Corresponding author: jitladda.sak@mahidol.ac.th*

Abstract

Natural rubber (NR) latex, derived from *Hevea brasiliensis*, is a critical biomaterial widely utilized in medical, industrial, and consumer applications due to its exceptional elasticity, barrier properties, and biodegradability. However, challenges such as allergenic proteins, batch variability, and environmental sustainability have necessitated extensive research to enhance its usability and industrial performance.

This presentation will delve into recent advancements in latex purification techniques, including deproteinization and saponification, which effectively remove allergenic proteins while maintaining the material's superior mechanical properties. The discussion will also explore novel strategies in latex stabilization and compounding, which address issues related to protein-induced hypersensitivity reactions and processing inconsistencies. Additionally, the lecture will highlight the role of NR latex in sustainable manufacturing, focusing on green processing technologies, life-cycle assessment, and its alignment with global sustainability frameworks such as the United Nations Sustainable Development Goals (SDGs).

This lecture will integrate polymer science, material engineering, and industrial applications to provide a comprehensive perspective on the transition of NR latex from a conventional raw material to a high-value, sustainable resource. The insights presented will be crucial for researchers, industry professionals, and policymakers striving to balance performance optimization with environmental responsibility in NR latex-based product development.

Keywords: Natural Rubber, Latex Purification, Allergen Reduction, Sustainable Manufacturing



Fig. 1 Scenarios of natural rubber latex from *Hevea* rubber tree to sustainable products

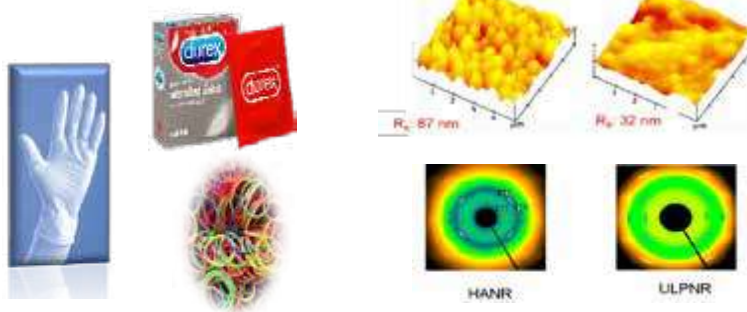


Fig. 2 Surface morphology from AFM analysis and WAXD patterns of HANR and ULPNR

MICROBIAL RUBBER DEGRADATION: NAVIGATING THE CHALLENGES FOR A SUSTAINABLE FUTURE

Kumar Sudesh

School of Biological Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia.

**Corresponding author: ksudesh@usm.my*

Abstract

Rubber waste, derived from both natural and synthetic sources, has become a significant environmental challenge due to its durability and resistance to degradation. Microbial degradation offers a promising, eco-friendly solution for addressing this issue. ¹ This presentation explores the potential of microbes in breaking down rubber, focusing on the mechanisms employed by bacteria and fungi, the challenges posed by rubber's chemical resistance, and recent advances in microbial engineering and enzyme optimization. Highlighting case studies on microbial degradation of tire waste ² and oceanic rubber particles, it emphasizes the role of interdisciplinary research and collaboration in overcoming barriers to scalability. ^{3,4} With the integration of microbial solutions ⁵ into waste management systems and policy frameworks, this approach holds immense potential for a sustainable future. This presentation will delve into the science, challenges, and opportunities in microbial rubber degradation for environmental restoration and innovation.

Keywords: Actinomycetes, biodegradable, microplastics, rubber

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ADVANCED FUNCTIONAL NANOCOMPOSITES OF NATURAL RUBBER AND SYNTHETIC POLYMERS: BRIDGING PERFORMANCE AND SUSTAINABILITY

**R Daik*, CY Lee, S Bidol, S Adnan, AA Shamsuri, HH Abd-Razak, HG Abdullah,
I Abdullah, MH Jumali, I Ahmad**

Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor,

**Corresponding author: rusli.daik@ukm.edu.my*

Abstract

The research focuses on nanocomposites of natural rubber (NR) and synthetic polymers, aiming to enhance their mechanical, thermal, and electrical properties while promoting sustainability. Liquid natural rubber (LNR) emulsions with molecular weights of 10,000 and 50,000 g/mol were prepared using sodium dodecyl sulphate (SDS) as an emulsifier. Emulsion droplet sizes were greater for LNR with higher molecular weight. LNR emulsions with lower molecular weight were more stable, requiring less emulsifier. Low-density polyethylene (LDPE)/LNR with compositions of 100LDPE/0LNR - 40LDPE/60LNR were created by mixing LDPE and LNR emulsions. The 60LDPE/40LNR composition provided optimal stress and strain values. Differential scanning calorimetry confirmed homogeneity in the blends with a consistent glass transition temperature. High-density polyethylene (HDPE)/LNR composites with modified montmorillonite (OMMT) were produced in compositions of 97/3 - 85/15, with 3% and 5% OMMT content. Thermal stability, tensile and impact strength improved with the addition of OMMT. X-ray diffraction and transmission electron microscopy revealed exfoliated structures at lower LNR content and mixed exfoliated-intercalated structures at higher LNR content. Nylon-6/LNR blends, with 2-10% OMMT, achieved improved tensile strength, hardness, and impact resistance at an optimal 85/15 ratio. Polycarbonate PC/LNR/OMMT nanocomposites with 2-10% OMMT exhibited increased thermal stability. Nanocomposites of polypyrrole (PPy) nanoparticles (11.91-36.25 wt%) in NR/polystyrene (PS) matrix demonstrated conductivities from 1.77×10^{-8} - 1.07×10^{-4} S/cm. Tensile strength (6.9-12.85 MPa) and Young's modulus (535-1279 MPa) improved with increasing PPy content. The research highlights how the incorporation of nanomaterials can tailor properties of natural rubber, aligning with industrial sustainability goals.

Keywords: Emulsion blending, low temperature processing, thermal conductivity, heat dissipation

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ADVANCEMENTS, MODIFICATIONS, AND TRENDS IN NATURAL RUBBER CHEMISTRY: FROM MOLECULAR INNOVATIONS TO PRACTICAL APPLICATIONS

Seng Neon Gan

Chemistry Department, University of Malaya

Corresponding author: sngan@um.edu.my

Abstract

Natural rubber, a *cis*-1,4-polyisoprene biopolymer, has evolved from its ancient Mesoamerican roots into a cornerstone of modern industry¹. The breakthrough of vulcanization reactions had converted NR into a durable material that fuelled the Industrial Revolution. Dry NR is produced by coagulating latex with acid. Major dry rubber products include tyres, belts, hoses and seals. Latex can be preserved for direct manufacturing². Key latex products include dipped goods, foams, coatings, carpet backing, and elastic threads. Chemical modifications of NR had led to changes in properties suitable for new applications³. Degradation of the NR could produce liquid rubbers of lower molecular weight and with reactive terminals⁴, for adhesive and blending with other materials. The 20th century saw strong competition from synthetic polymers, yet NR retained its dominance in critical applications. In the 21st century, scientists have placed more efforts on environmental protections and energy saving techniques that included developing biodegradable composites, and compounds with less toxic accelerators and additives. A notable example is the replacement of carcinogenic aromatic oil in tyre manufacturing with palm oil-based polyester⁵. Another example is the used of silica from rice husk to replace carbon black⁶ as filler. In recent years, rubber glove industry has accounted for more than 50% of NR latex usage. There are two major challenges: (i) protein allergy and (ii) donning problem. One of reported approach to the first problem is by carrying out emulsion polymerization of diethylaminomethyl methacrylate (DMAEMA) in latex, which results in the grafting of poly(DMAEMA) onto the latex particles, and displacing the allergenic protein⁷. The second problem is due to the surface tackiness of rubber. Several methods have been reported, these include the use of powder, flocking, chlorination, and polymer coating⁸. Through continuous molecular innovations, NR remains indispensable, adapting to global challenges while expanding its application frontier.

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DIRECT OBSERVATION OF BOTH FORMATION AND DEGRADATION OF RUBBERS BY ELECTRON SPIN RESONANCE (ESR)

Atsushi Kajiwarara

Nara University of Education, JAPAN

*Corresponding author: kajiwarara@cc.nara-edu.ac.jp

Abstract

Whether plastics or rubber materials, interest has focused on the chemistry of the starting materials and products. Many of these materials are produced by radical polymerization. In recent years, the sensitivity of electron spin resonance (ESR) spectroscopy has improved, making it possible to directly observe radicals, the active species in the course of a reaction, by ESR, which could not be observed before¹⁾. In combination with pulsed lasers, it has also become possible to observe the very early stages of reactions. The direct observation of radicals provides direct experimental evidence of the reaction process, which previously could only be inferred²⁾. An example is shown in Figure 1. This is the result of ESR observation of the radical polymerization of isoprene. The time-resolved ESR method shows that the initial stages of polymerization can be observed in the high-resolution spectrum of isoprene propagating radicals in steady-state ESR. Since isoprene is an asymmetric diene, the analysis of the spectrum provides information on the direction of radical addition and the detailed structure of the propagating radicals formed. 1,3-Butadiene and Isoprene are important raw materials for synthetic rubber. Their polymerization reactions can be studied in detail by ESR. Copolymers of butadiene with styrene or acrylonitrile are also important synthetic rubbers, and their copolymerization reactions can also be studied by ESR. Not only the reaction, but also the physicochemical properties of the resulting rubber material can be observed by ESR. When rubbers are artificially stretched, the covalent bonds of the constituent polymers are broken, and radicals are generated. These radicals can be observed by ESR. Since pyrolysis and photolysis of rubber materials also break covalent bonds in both cases, the radicals produced by the breakage can be observed and the details of the decomposition reaction can be determined.

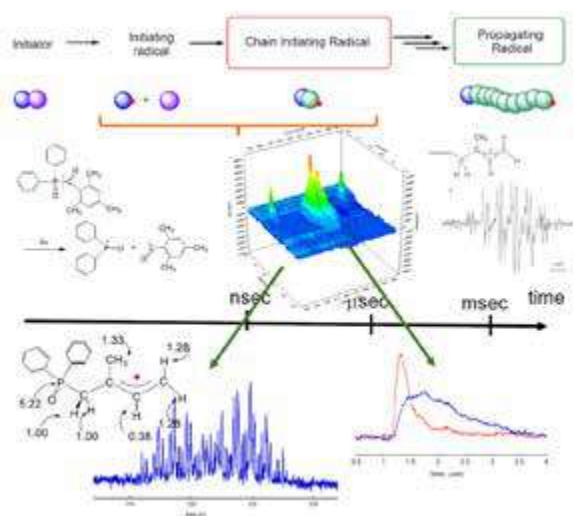


Figure 1: Time-resolved ESR and steady-state ESR observation of radical polymerization of isoprene. Both chain initiating and propagating radicals can be observed in the same polymerization system.

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ECO-FRIENDLY SYNTHESIS OF CROSSLINKED MICROSPHERES FROM EPOXIDIZED NATURAL RUBBER LATEX TOWARD SUSTAINABLE POLYMER DEVELOPMENT

M. Siti Nor Qamarina^{a,*}, A. Nurulhuda^a

^aTechnology and Engineering Division, Malaysian Rubber Board, 47000, Sungai Buloh, Selangor, Malaysia

*Corresponding author: qamarina@lgm.gov.my

Abstract

Synthesis of crosslinked microspheres from petroleum-based resources has raised considerable sustainability awareness. Therefore, bio-based polymers have been identified as viable alternatives, including epoxidized natural rubber latex (ENRL).¹ ENRL is predominantly employed within the rubber goods industries, and extending its use beyond conventional usage represents a novel approach. Herein, the development of crosslinked microspheres was accomplished by leveraging the epoxide and vinyl features in the polymer backbone by ring-opening and free-radical polymerization, correspondingly, with both reactions performed in an aqueous environment. The epoxide ring-opening of ENRL with maleic anhydride (MA), an environmentally friendly crosslinking agent,^{2,3} has efficiently installed ester crosslinking between ENRL polymer chains, evidenced by the transition of ENRL from liquid to paste-like consistency, corroborated by nuclear magnetic resonance (NMR), Fourier transform infrared (FTIR) and microscopy analyses. Vinyl functionalization of ester-crosslinked ENRL microspheres was successfully performed through free-radical polymerization using 3-(trimethoxysilyl)propyl methacrylate (TMSPMA) monomer.^{4,5} The inorganic-hybridized microspheres synthesized were in a form of free-flowing powder. These hybrid microspheres were interpreted as having soft and flexible properties in the core, while exhibiting solid and durable attributes at the outermost layer. Their robust structural integrity renders them outstanding in solvent stability, thereby conferring these novel microspheres as a potential precursor for advanced material applications.

Keywords: Epoxidized natural rubber latex (ENRL), ring-opening reaction, free-radical polymerization, paste-like consistency, hybrid microspheres

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RESOLVING THE MICROSTRUCTURE OF NATURAL RUBBER AND ITS INFLUENCE ON THE MECHANICAL PROPERTIES

Jinrong Wu^{a,*}

^a National Key Laboratory of Advanced Polymer Materials, College of Polymer Science and Engineering, Sichuan University, Chengdu, Sichuan, 610065

*Corresponding author: wujinrong@scu.edu.cn

Abstract

Natural rubber (NR) serves as a critical elastic material in aerospace, defense, and automotive applications, owing to its superior overall characteristics. In recent years, we have elucidated the multiscale structural organization of pre-vulcanized natural rubber latex films (VNRL) and compared it with vulcanized natural rubber sheets (VNR) fabricated through mechanical blending and compression molding. While both materials share equivalent total crosslink density, VNRL displays a structurally uniform network enriched with molecular entanglements compared to VNR. Although this enhanced entanglement density initially retards strain-induced crystallization (SIC) and reduces crystallinity in moderate strain regimes relative to VNR, VNRL demonstrates accelerated crystallization kinetics at elevated strains. This enhancement arises from the formation of larger crystallites, enabling VNRL to surpass VNR in crystallinity at high strains. The homogeneous architecture of VNRL further facilitates greater network extensibility, yielding superior ultimate tensile strain and fracture strength. Based on these insights, a non-invasive latex-phase processing strategy has been devised to fabricate high-performance rubber materials with highly entangled, homogeneous, and low-defect networks. NR products manufactured via this innovative method retain native chain entanglements while achieving enhanced structural uniformity and reduced defects. The refined network architecture improves SIC of NR, attaining crystallinity levels up to 38% alongside increased crystal dimensions. These structural optimizations lead to markedly improved mechanical performance, substantially exceeding that of conventionally processed NR materials.

Keywords: Natural rubber; Strain-induced crystallization; Network structure

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Beyond Isocyanates: Charting the Course for Green Polyurethane in Rubber and Latex

Siang Yin LEE^{a*}, Rhun Yian KOH^b

^a*Technology and Engineering Division, RRIM Sungai Buloh Research Station, Malaysian Rubber Board, 47000 Sungai Buloh, Selangor, Malaysia.*

^b*School of Health Sciences, International Medical University, No. 126, Jalan Jalil Perkasa 19, Bukit Jalil, Kuala Lumpur 57000, Malaysia.*

**Corresponding author: leesiangyin@lgm.gov.my*

Abstract:

The development of non-isocyanate polyurethane (NIPU) offers a safer and more sustainable alternative to conventional polyurethane (PU) by eliminating hazardous isocyanates from the production process. This presentation explores the synthesis, characterization, and industrial potential of palm-based NIPU, highlighting its advantages and challenges in rubber, latex, and adhesive applications. A series of palm-derived NIPU was synthesized through the polyaddition of cyclic carbonates with diamines, in the presence of palm-based derivatives. Cytotoxicity evaluations confirmed their non-toxic nature, with cell viability exceeding 80%. Thermal characterization revealed glass transition temperatures (-10°C to 50°C) and decomposition stability (230°C – 270°C), ensuring suitability for high-performance applications. Mechanical assessments demonstrated the potential of NIPU in carbon black masterbatch, where tensile strength ranged from 15–20 MPa, with crosslink density and hardness (Shore A) in the range of 60–70. Similarly, NIPU-modified latex films exhibited tensile strengths of 15–23 MPa, making them viable for flexible coatings and dipped goods. Despite its advantages, barriers to large-scale adoption remain, including processing challenges and viscosity limitations. This presentation will discuss strategies to enhance NIPU formulation and scalability, aiming to bridge the gap between research advancements and commercial viability. By optimizing the NIPU properties and industrial integration, this work contributes to the development of sustainable, bio-based palm-based NIPU materials for potential diverse industrial applications.

Keywords: Non-isocyanate polyurethane; Palm-based NIPU; Cytotoxicity; Rubber; Latex.

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BIODEGRADABLE ANTIMICROBIAL LATEX FILMS FOR STETHOSCOPE DIAPHRAGM COVERS VIA LATEX DIPPING PROCESS

Neettha Nai Sem¹, Muhammad Khalil Abdullah¹, Husnul Azan Tajarudin²,
Azura A. Rashid^{1*}

¹ *School of Materials and Mineral Resources Engineering, Universiti Sains Malaysia,
Engineering Campus, 14300 Nibong Tebal, Seberang Perai Selatan,
Pulau Pinang, Malaysia.*

² *School of Industrial Technology, Universiti Sains Malaysia, 11800 Gelogor, Penang, Malaysia.*

**Corresponding Author: srazura@usm.my*

Abstract

A disposable stethoscope diaphragm cover provided a hygienic barrier against nosocomial pathogens, thus reducing the transmission of microbes. In this work, natural rubber (NR) and polyisoprene (PI) latex films were filled with zinc oxide nanoparticles (ZnO NPs) and mangosteen peel powder (MPP) to investigate their antimicrobial properties and mechanical performance. The research also included the design of a novel stethoscope former for dipping the antimicrobial latex stethoscope covers. The stethoscope cover was designed using SolidWork™ software and fabricated via 3D printing using Polylactic Acid (PLA) at 200°C. The metal former was duplicated based on the 3D-printed former and subjected to a dipping process. The parameters, such as temperature, speed, curing rate, and leaching, were recorded to determine optimal conditions in producing latex films. The tensile properties and antimicrobial activity were investigated, and results were recorded. An antimicrobial loading of 1.0 phr was incorporated into NR and PI latex compounds to evaluate their effectiveness in inhibiting bacterial and fungal growth. MPP showed the highest efficacy with the largest inhibition zone, while ZnO NP demonstrated strong antimicrobial activity in both NR and PI latex. The addition of these agents had a similar impact on the mechanical properties of the latex films. NR films with antimicrobial agents exhibited improved tensile strength and elongation at break compared to the control (29.41 MPa, 1353%), MPP (33.84 MPa, 1351%) and ZnO NP (31.79 MPa, 1386%). Similarly, PI latex films showed enhanced tensile strength and elongation at break of ZnO NP (22.18 MPa, 1274%) and MPP (24.57 MPa, 1413%), compared to the control (21.61 MPa, 1468%). ZnO NP proved a promising option due to its dual functionality as an activator and an antimicrobial agent. This study underscores the potential of antimicrobial latex stethoscope covers to enhance infection control in medical settings.

Keywords: Antimicrobial agents, Natural Rubber (NR) latex, Polyisoprene (PI) PI latex, stethoscope diaphragm cover mold, 3D Printing.

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EVALUATION OF RECOVERED CARBON BLACK IN WET NATURAL RUBBER MASTERBATCH: COMPARISON OF PHYSICAL, DYNAMIC PROPERTIES, AND PRODUCT PERFORMANCE WITH COMMERCIAL CARBON BLACK

**Siti Salina Sarkawi, Teku Zakwan Zaeimoedin, Nurul Hayati Yusof, Ahmad Kifli Che Aziz,
Nik Intan Nik Ismail, Nor Hidayaty Kamarulzaman, Kamarularifin Hadithon and
Yusniwati Mohamed Yusof**

*Technology and Engineering Division
Malaysian Rubber Board, 47000, Sungai Buloh, Selangor, Malaysia
#Corresponding author: ssalina@lgm.gov.my*

Abstract

This research investigates the potential of recovered carbon black (rCB) derived from end-of-life tires as a sustainable reinforcing filler in wet natural rubber (NR) masterbatch formulations, comparing its performance with conventional commercial carbon black (CB). The wet masterbatching technique was employed to enhance filler dispersion and reduce energy consumption during rubber processing. Comprehensive evaluations of the physical and dynamic properties were conducted, including tensile strength, modulus, elongation at break, hardness, and abrasion resistance, to assess the mechanical performance. Dynamic mechanical analysis (DMA) provided insights into viscoelastic behavior, focusing on parameters such as storage modulus, loss tangent, rolling resistance, and wet grip potential. Additionally, the end-use performance of rubber products incorporating rCB was tested under application-specific conditions and benchmarked against CB-based products. The findings reveal that rCB can offer comparable mechanical reinforcement and dynamic properties, with certain trade-offs in performance depending on the specific application requirements. This study highlights the potential of rCB as a sustainable alternative for the rubber industry, contributing to waste valorization and the advancement of circular economy initiatives.

INFLUENCE OF VISCOSITY AND RUBBER VARIANTS ON THE MOLECULAR CHARACTERISTICS OF NATURAL RUBBER DEPOLYMERIZATION

Krishna Veni Baratha Nesan^a, Nik Intan Nik Ismail^a,

^a Malaysian Rubber Board, 47000, Sungai Buloh, Selangor, Malaysia

*Corresponding author: krishnaveni@lgm.gov.my

Abstract

The depolymerisation of natural rubber (NR) is significantly influenced by processing conditions, particularly viscosity and the type of rubber used¹². This study investigates the influence of Mooney viscosity using SMR20 as a model material, while also evaluating the molecular degradation characteristics across five NR variants—SMR10, SMR20, SMRL, DPNR, and RSS. The Mooney viscosity of SMR20 was varied through controlled mastication to understand its impact on the molecular weight reduction during depolymerization³. Subsequently, all five rubber types were subjected to identical depolymerisation conditions to assess the effect of non-rubber constituents and dirt content on degradation efficiency⁵⁶.

The depolymerised NR samples were characterised using Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TGA), and Gel Permeation Chromatography (GPC). Results revealed that a reduction in Mooney viscosity in SMR20 correlated with a progressive decrease in weight-average molecular weight (Mw) and narrowing of molecular weight distribution (PDI), indicating efficient chain scission³. Comparative analysis of different NR types showed distinct degradation behaviours, primarily attributed to the presence of non-rubber components such as proteins, lipids, and dirt⁵⁶. For example, SMRL and RSS, which typically contain higher impurities, showed lower degradation efficiency than more refined grades like DPNR and SMR10.

Thermal analysis demonstrated improved thermal stability in more uniformly degraded NR samples, while spectroscopic analysis confirmed the formation of functional end groups such as carbonyl and hydroxyl that are beneficial for downstream modification and reactivity¹². These findings highlight the critical roles of initial viscosity and rubber purity in determining depolymerisation outcomes. Optimising these factors can lead to more controlled synthesis of depolymerised NR, enhancing its applicability in adhesives, coatings, thermoplastic blends, and reactive polymer systems⁴.

Keywords: Liquid Natural Rubber (LNR), Depolymerization, Mooney Viscosity, Natural Rubber Variants, Molecular Weight Distribution

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IMPACT OF RRIM HYDROBEST™ AND MORTEX STIMULANTS ON LATEX PROPERTIES IN PB350 CLONE RUBBER TREES: A COMPARATIVE STUDY

Dazylah Darji **, Mohamad Akmal Abdul Rahim*, Nurul Hayati Yusof*, Shaikh Mohd Hizami Shaikh Abd Hadi*, Nik Intan Nik Ismail*, Muhammad Syaarani Danya*, Muhammad Akbar Abdul Ghaffar*

**Rubber Research Institute of Malaysia, Malaysian Rubber Board, 47000 Sungai Buloh, Selangor, Malaysia
Corresponding author: dazylah@lrm.gov.my*

Abstract

This study examines the effect of stimulant application, specifically RRIM HYDROBEST™ and Mortex derived from clone PB350, in RRIMINIS Seri Iskandar, Perak. This trial was designed to investigate the effects of two types of stimulants on PB350 clone trees tapped with the suggested tapping system (d3) with and without stimulation. Field latex parameters were measured, including total solids content (TSC), dry rubber content (DRC), viscosity, particle size, nitrogen content, molecular weight, and volatile fatty acid (VFA). The control group (unstimulated) had greater TSC and DRC values than the stimulated RRIM HYDROBEST™ and Mortex. The usage of stimulants resulted in decreased viscosity and molecular weight. While stimulated latex has slightly reduced the latex particles compared to unstimulated latex. The decreased viscosity, molecular weight, and particle size of stimulated latex are due to increased metabolic activity and dilution by additional fluids secreted by the tree. Nitrogen content was found to be significantly higher in the rubber from stimulated latex compared with that in from unstimulated latex. It is interesting to note that Mortex-stimulated latex had higher VFA than RRIM HYDROBEST™ and unstimulated latex.

Keywords: latex properties, stimulant, RRIM HYDROBEST™, Mortex



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RECYCLING EPDM MOLDED FLASH THROUGH CONTINUOUS THERMO-MECHANICAL DEVULCANISATION

Nik Intan Nik Ismail^a, Siti Salina Sarkawi^a, Hani Afiffa Mohd Hanif^a, Nurul Hayati Yusof^a and Dayang Habibah Abang Ismawi Hassim^a

^a*Technology and Engineering Division
Malaysian Rubber Board, 47000, Sungai Buloh, Selangor, Malaysia.*

**Corresponding author: nikintan@lgm.gov.my*

Abstract

Ethylene Propylene Diene Rubber (EPDM) is a commonly used synthetic rubber in automotive parts, roofing, seals, and gaskets due to its excellent resistance to heat, ozone, and weathering. However, excessive flashes from the moulding line can achieve up to 30%, which is a significant loss for a manufacturer of dry rubber products. This study focuses on recycling EPDM flash and reusing the recycled material as filler or rubber replacement up to 80% in EPDM compound. The rubber recycling was performed in a co-rotating twin-screw extruder at different barrel temperatures, ranging from 180 to 220 °C, with variation screw speed from 50 to 120 rpm to determine the optimised recycling parameters. The recycled EPDM powders were analysed via thermogravimetric analysis (TGA), Scanning Electron Microscopy (SEM) and Dynamic Mechanical Analysis (DMA) to understand its degradation characteristics after the thermo-mechanical process. Furthermore, Fourier Transform Infrared (FTIR) Spectroscopy was performed to provide an insight into the chemical changes in the devulcanised recycled EPDM. The recycled EPDM processed under 180 °C with 120 rpm showed more prominent reduction of sulfur crosslink peaks at 531, 711 and 1058 cm⁻¹, relating to S-S, C-S and S-O bonds, respectively¹⁻² [Figure 1]. To assess the processability of the recycled EPDM, the powder was mixed and revulcanised. The quality of the revulcanised blend was measured based on rheometer, tensile strength, modulus and hardness. Results suggest that the EPDM waste could be recycled into new competitive products with low energy consumption. The findings would benefit the rubber industry by supporting dry rubber products' circular economy and end-of-life cycle.

Keywords: recycling EPDM, thermo-mechanical devulcanisation and circular economy.

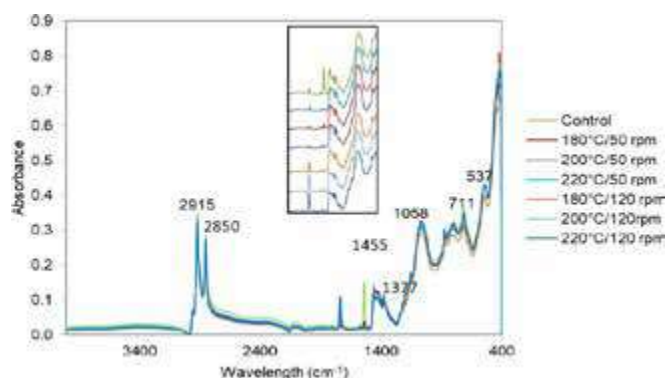


Figure 1. Spectral regions between 4000 and 400 cm⁻¹ of the recycled EPDM and control

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SUSTAINABLE COMPOUNDING: INNOVATIONS IN GREEN INGREDIENTS FOR THE RUBBER INDUSTRY

Nadras Othman^{1*}, Muhamad Sharan Musa², Nabil Hayeemasae³, Şehriban Öncel⁴, Bağdagül
Karaağaç⁵, Nur Raihan Mohamed⁶

^{1,2}*School of Material and Mineral Resources Engineering, Universiti Sains Malaysia, Engineering Campus, 14300 Nibong Tebal, Penang, Malaysia;* ³*Department of Rubber Technology and Polymer Science, Faculty of Science and Technology, Prince of Songkla University, Pattani Campus, 94000, Pattani, Thailand,* ^{4,5}*Department of Chemical Engineering, Umuttepe Campus, Kocaeli University, 41001 Kocaeli, Türkiye,* ⁶*Faculty of Applied Sciences, University Teknologi MARA, Perlis Branch, 02600 Arau, Perlis, Malaysia*

**Corresponding author; srnadras@usm.my*

Abstract

The rubber industry, facing increasing environmental scrutiny and resource limitations, is actively seeking sustainable alternatives to conventional compounding practices. This review explores recent innovations in green ingredients that offer promising pathways towards a more environmentally responsible rubber manufacturing sector. The focus lies on the development and application of bio-based fillers, such as agricultural waste and lignocellulosic materials, which can partially or fully replace traditional carbon black and silica, reducing reliance on fossil resources and minimizing greenhouse gas emissions. Furthermore, advancements in bio-based plasticizers and processing aids derived from renewable sources like vegetable oils and natural resins are examined for their potential to enhance rubber performance while lowering the environmental impact associated with conventional petroleum-based additives. The integration of these green ingredients necessitates innovative compounding techniques and processing methodologies to ensure comparable or improved material properties and processability. This review highlights the potential of sustainable compounding strategies to not only address environmental concerns but also to create new value streams and enhance the long-term viability of the rubber industry. The performance and environmental advantages of these cutting-edge green chemicals will be reviewed based on recent study findings.

NATURAL RUBBER LATEX (NRL) WASTE EFFLUENT AND *HEVEA* PROTEIN PURIFICATION: A MICROSCOPIC STUDIES

Hairani Tahir

Department of Polymer technology, School of Industrial Technology, Faculty of Applied Sciences Universiti Teknologi MARA Shah Alam, Selangor Malaysia.

**Corresponding author: haira331@uitm.edu.my*

Abstract

NRL waste effluent were collected to extract *hevea* protein and the application studies were investigated to give some reputation to this well-known allergen in latex product industry. The use of this *hevea* protein was proposed on metal removal and antimicrobial activities and yet metal removal was found more profound. Investigation on the microscopic level was conducted to have a good understanding on the physical characteristics of the NRL serum alongside with the 15-identified protein. These proteins serve various functions from the biosynthesis of polyisoprene to protection of rubber tree against fungicide as well as formation of protective layer to help wound healing after each tapping. Each treatment to purify waste serum to isolates the protein was investigated using HRTEM to observe the microscopic image of the rubber particle and *hevea* protein. The images captured also showed how metal binding occurred at the microscopic level which indicates heavy protein also works well even without intense purification. Among all the proteins in the serum, there are numbers of it that have potential to be highlighted. This study provides fundamental knowledge on *hevea* protein role supported by microscopic images.

Keywords: waste, *hevea* protein, microscopic

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CATECHIN-RICH UNCARIA GAMBIR AS A DUAL-FUNCTION ANTIOXIDANT AND CO-CROSSLINKING AGENT IN NATURAL RUBBER LATEX FILMS

Hakimah Osman^{a*}, Zunaida Zakaria^a, Nor Azura Abdul Rahim^a, Teh Pei Leng^a

^a Faculty of Chemical Engineering & Technology, Universiti Malaysia Perlis (UniMAP), Perlis, Malaysia.

*Corresponding author: hakimah@unimap.edu.my

Abstract:

A comparative investigation was conducted on a natural antioxidant derived from *Uncaria gambir* (NAO) and a commercial phenolic antioxidant (CAO) to assess their effects on the properties of pre-vulcanized natural rubber latex (NRL) films. This study aimed to evaluate the dual functionality of NAO as both an antioxidant and a potential co-crosslinking agent in rubber compounding. Key parameters analyzed included particle size distribution, compounding viscosity, mechanical stability, tensile properties, crosslink density, and thermal ageing behavior. From a chemical perspective, *Uncaria gambir* is rich in catechin, a polyphenolic compound containing multiple hydroxyl groups capable of scavenging free radicals, thereby inhibiting oxidative degradation. These hydroxyl groups also provide reactive sites that may participate in crosslinking reactions during vulcanization, either through electrophilic aromatic substitution or oxidative mechanisms involving quinone intermediates. Such interactions may form covalent bonds with unsaturated polyisoprene chains, enhancing network formation and thermal resilience. Experimental findings revealed that NAO possessed a smaller average particle size (20.3 μm) than CAO (23.5 μm), facilitating superior dispersion and interaction with the rubber matrix. Although both antioxidants influenced viscosity and mechanical stability, NAO-enhanced films demonstrated improved tensile strength, elongation at break, and modulus, particularly before and after thermal ageing. FTIR analysis confirmed the stability of the phenolic functional groups in NAO post-ageing, indicating structural integrity. While NAO exhibited slightly lower crosslink density than CAO, its superior retention of mechanical properties and thermal stability underscores its potential as a sustainable dual-function additive. These results support the application of *Uncaria gambir* as a green alternative to synthetic antioxidants, contributing to the development of environmentally friendly, high-performance rubber materials.

Keywords: *Uncaria gambir*, Catechin, Natural rubber latex, Antioxidant, Co-crosslinker

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A COMPARATIVE STUDY OF ANALYTICAL METHODS FOR PHTHALATE DETERMINATION IN TOYS AND CHILDCARE PRODUCTS

Zatil Afifah Omar, Fauzi Mohd Som

Quality and Technical Services Division

Malaysian Rubber Board, 47000, Sungai Buloh, Selangor, Malaysia

#Corresponding author: zatil.affah@lgm.gov.my

Abstract

Phthalates are commonly used as plasticizers in elastomeric materials, particularly in consumer products such as toys and childcare products. Due to their potential health risks, various international regulatory bodies have established standardized methods for their detection and quantification. This study compared two widely used international standards for phthalate testing, CPSC-CH-C1001-09.4 (Standard Operating Procedure on Determination of Phthalates) and IEC 62321-8 (Determination of certain substances in electrotechnical products - Part 8: Phthalates in polymers by gas chromatography-mass spectrometry (GC-MS), gas chromatography-mass spectrometry using a pyrolyzer/thermal desorption accessory (Py-TD-GC-MS)), focusing on their sensitivity, selectivity, and overall analytical performance. Key parameters such as peak resolution, signal-to-noise ratio, matrix effects, and detection limits were evaluated using spiked elastomer samples. The results indicated that both methods are effective in detecting regulated phthalates, but differences in selectivity and sensitivity may influence method suitability for specific applications. This comparative analysis provided insights into the strengths and limitations of each approach, aiding in the selection of an appropriate method for regulatory compliance and routine quality control in toys and childcare products.

Keywords: Phthalates, Elastomers, Analytical Methods, Regulatory Standards, CPSC-CH-C1001-09.4, IEC 62321-8, Sensitivity, Selectivity

ANALYSIS ON TREATED RECOVERED CARBON BLACK (RCB) FILLER AND THEIR PERFORMANCE IN RUBBER COMPOUNDS FOR SUSTAINABLE PRODUCT APPLICATIONS

Teku Zakwan Zaeimoedin,^{a,#} Kamarularifin Hadithon^a, Siti Salina Sarkawi^a, Ahmad Kifli Che Aziz^a, Nik Intan Nik Ismail^a and Nor Hidayaty Kamarulzaman^a.

¹ *Technology and Engineering Division*

Malaysian Rubber Board, 47000, Sungai Buloh, Selangor, Malaysia

[#]*Corresponding author: zakwan@lgm.gov.my*

Abstract

Recovered carbon black (rCB) has emerged as a sustainable alternative to traditional carbon black filler in the rubber industry. The recovered carbon black (rCB) that thermochemically recovered from end-of-life tyres, has already made the leap into industrial practice, and is making an important contribution to closing the loop in the tyre and rubber industry in the world. The first Cradle to Cradle certificate for rCB was already issued by EPEA in 2017, and most recently another rCB was accredited under the International Sustainability & Carbon Certification (ISCC) scheme. Besides the environmental advantages of using rCB in the rubber & tyre industry, for instance that of CO₂ reduction, the economic feasibility of pyrolysis is positively affected by these markets. These recovered carbon black (rCB), can be reintroduced in rubber industry as filler (circular economy concept) and giving an alternative carbon black fillers to rubber industry. Acid and base demineralization processes (chemical upgrading) seem to be imperative because inorganic compounds are practically unavoidable in the rCB, while surface chemistry is strongly dependent of the pyrolysis conditions. In this research the rCB was treated with HCL at 10% concentration (w/w) for 8 hours at room temperature. The mixture was then filtered through PTFE paper, rinsed with sodium hydroxide, and dried in a convection oven at 60 °C. The treated rCB samples then, were analysed using scanning electron microscope (FESEM), BET analyzer for the morphology of rCB and thermogravimetry analyzer for the materials composition in the rCB in order to determine the effectiveness of the treatment process. The assessment on the performance and properties of these rCB filler in rubber compound for rubber products application also have been evaluated and compared with the commercial carbon black. From the BET surface area results obtained, the treated rCB surface area increased from 70.3759 m²/g to 78.6374 m²/g and showed similar BET surface area to N330 carbon black. While in term of material composition by using TG analysis on the treated rCB, the carbon black content % increased from 78% to 83% as well as reduced the ash content from 14.4% to 9.5%. The increase in BET surface area and carbon black content % in the treated rCB can influenced the reinforcing effect of rCB filler in the rubber compound for the rubber product applications.

Keywords: recovered carbon black; end-of-life tyre; pyrolysis, sustainability; and circular economy.

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JOURNAL OF RUBBER RESEARCH SPECIAL ISSUE: ADVANCING SUSTAINABLE NATURAL AND SYNTHETIC RUBBER OR LATEXES TECHNOLOGIES FOR TOMORROW

Veronica Charlotte

Publications and Library, Support Services Division, Malaysian Rubber Board, 148, Jalan Ampang, Kuala Lumpur, 50450, Malaysia.

**Corresponding author: veronica@lgm.gov.my*

Abstract

In celebration of its century of innovation and partnership, the Malaysian Rubber Board (MRB) is proud to announce a forthcoming Special Issue (SI) of the Journal of Rubber Research (JRR), a Scopus-indexed SpringerLink journal. This special publication, titled “Advancing Sustainable Natural and Synthetic Rubber or Latexes Technologies for Tomorrow,” coincides with the “IKM-MRB Symposium on Elastomers and Latexes (IMSEL 2025),” co-organized by the MRB and the Malaysian Institute of Chemistry (IKM) as part of the 50th World Chemistry Congress (50WCC) under IUPAC 2025. The JRR is a distinguished peer-reviewed publication that delves into all aspects of natural and synthetic rubbers and their related disciplines. Its comprehensive scope spans core areas such as biology, physics, chemistry, and economics, focusing on active experimental research and authoritative reviews. The journal serves as a vital platform for building a collective knowledge base, disseminating information, and validating the quality of research within the rubber science community. It is a central hub for experts across academia and industry engaged in rubber research and applications, providing both a valuable source of information and a prestigious avenue for their publications. The upcoming JRR-SI specifically seeks to highlight innovative and value-added research that contributes to the advancement of sustainable technologies in natural and synthetic rubber and latexes. Submissions are encouraged across the entire spectrum of rubber science, encompassing upstream, midstream, and downstream aspects, with a particular emphasis on biology, physics, and chemistry. This initiative aims to showcase cutting-edge research and foster crucial discussions that will drive the future progress of the latex and rubber industry.

Keywords: Natural rubber, Synthetic rubber, Latex, Sustainable technologies, Rubber industry

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DEVELOPMENT OF A NATURAL RUBBER LATEX WITH PALM-OIL BASED NON-ISOCYANATE POLYURETHANE-ACRYLATE PLASTICISER

Ki Yan Lam^a, Choy Sin Lee^{a*}, Yun Khoon Liew^b, Siang Yin Lee^c, Jia Yu Ng^d, Ying Hong Lim^d
and Suvashyree A/P Rajagopal^d

^a*Department of Pharmaceutical Chemistry, School of Pharmacy, IMU University, No. 126, Jalan Jalil Perkasa 19, Bukit Jalil, 57000 Kuala Lumpur, Malaysia.*

^b*Department of Life Science, School of Pharmacy, IMU University, No. 126, Jalan Jalil Perkasa 19, Bukit Jalil, 57000 Kuala Lumpur, Malaysia.*

^c*Colloids and Interface Science Centre (CISC), Centre of Excellence (COE), RRIM Sungai Buloh Research Station, Malaysian Rubber Board (MRB), 47000 Sungai Buloh, Selangor, Malaysia*

^d*School of Pharmacy, IMU University, No. 126, Jalan Jalil Perkasa 19, Bukit Jalil, 57000 Kuala Lumpur, Malaysia.*

*Corresponding author: choysin_lee@imu.edu.my

Abstract

Natural biomaterials have gained great attention, particularly for their versatility in biomedical applications due to their biodegradability, mechanical flexibility and ability to be tailored for specific functions. Among these, natural rubber latex (NRL) stands out for its exceptional elasticity, durability, and barrier properties, making it highly suitable for medical gloves, tubing, catheters, wound dressings, and other healthcare-related products.¹ In the NRL formulation, plasticiser is one of the key components in improving physical properties of NRL. Traditionally, petroleum-based mineral oils have been used as plasticisers but they are non-renewable and contained high level of polyaromatic hydrocarbon, which poses carcinogenic risks.² This has driven the demand for greener alternatives that not only improve rubber performance but also align with sustainability goals in biomedical material development. In this study, a palm oil-based non-isocyanate polyurethane-acrylate was used as a plasticiser in the dry natural rubber (DNR) formulations. The performance of this palm oil-based plasticiser was compared with commercial plasticiser (Tudalen 65) and unplasticised DNR. The resulting DNRs were characterised by differential scanning calorimetry, thermogravimetric analysis and tensile strength tests. The NRL with palm-oil plasticiser exhibited comparable mechanical properties with both blank DNR and DNR with a commercial plasticiser, with elongation at break exceeding 720% and tensile strength of ~30 MPa. Thermal analysis revealed that the palm oil-based plasticiser improved thermal stability of the DNR with two distinct glass transition temperatures. In biodegradability assessment, the DNR prepared by palm oil-based plasticiser was less susceptible to microbial degradation compared to blank DNR but was similar to the commercial plasticiser. Under elevated temperature, the DNR prepared by palm oil-based plasticiser exhibited a 2-fold weight loss in hydrolytic degradation compared to other samples. These findings demonstrate the potential of palm-oil-based plasticisers as a sustainable alternative for DNR, offering comparable mechanical and improved thermal and hydrolytic degradation properties to conventional plasticisers.

Keywords: Palm oil, plasticiser, biomaterial, dry natural rubber

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ZERO-WASTE CLOSE-LOOP BIOREFINERY SYSTEM FOR FOOD AND YARD WASTE VALORIZATION

**Jinhua Mou^{1,2}, Yahui Miao¹, Ziyao Liu¹, Di Wu¹, Jiale Zhu^{1,3}, Sun Zheng³, Xiang Wang⁴,
Peizeng Yang¹, Zhenyao Wang¹, Shao-Yuan Leu⁵, Chunbao Xu¹, Sze Ki Carol Lin^{1,*}**

¹*School of Energy and Environment, City University of Hong Kong, Kowloon, Hong Kong*

²*College of the Environment & Ecology, Xiamen University, China*

³*College of Fisheries and Life Science, Shanghai Ocean University, Shanghai, 201306, China*

⁴*Key Laboratory of Eutrophication and Red Tide Prevention of Guangdong Higher Education Institutes, College of Life Science and Technology, Jinan University, Guangzhou 510632, China*

⁵*Department of Civil and Environmental Engineering, The Hong Kong Polytechnic University, Hong Kong SAR, China*

**Corresponding author: carollin@cityu.edu.hk*

Abstract

According to Hong Kong Environmental Protection Department (HKEPD), approx. 1.2 million ton food waste (FW) and 80 kilo ton yard waste (YW), as two typical organic solid wastes, are generated annually in Hong Kong. In fact, both FW and YW are valuable renewable carbon resources or green alternatives to petroleum for energy and chemical production. However, the majority of these resources in Hong Kong are disposed of as wastes at landfills or by incineration, causing not only fast-depleted landfill spaces, but also secondary pollutions (leachate, CH₄ GHG, NO_x, and dioxins). Therefore, it is urgent to develop new technologies for the harmless, reduction, and resourceful treatment of organic wastes for bioenergy and high value-added bioproducts, in order to achieve the goal of zero landfill by 2035 & carbon neutrality by 2050 in the Hong Kong and support China's initiative of promoting the construction of "waste-free cities". Previous efforts in conversion of biomass or organic solid waste (OSW) often focused primarily on specific target bioproducts, but they often overlooked the potential of valorization of the byproducts generated during the biomass/OSW conversion process. In this talk, we will cover three recent research projects which are related to the development of innovative biorefinery approach for conversion of FY & YW into multiple high value-added bioproducts, namely biobased non-isocyanate polyurethane (NIPU) resin and sustainable aviation fuel. The first part of the talk will focus on utilizing the obtained food waste lipids (FWLs) as a promising feedstock for producing a bioplastic: non-isocyanate polyurethane (NIPU) resin, potentially aiding in the mitigation of plastic pollution. The objective of is to develop a green and novel production pathway of fully bio-based NIPU resins from FWLs with the incorporation of CO₂ fixation. The second part of the talk will focus on the fermentative production of 2,3-butandiol (2,3-BDO) using novel bacterial strains OPS2 and subsequently the iso-alkanes SAF components from the cellulose-rich substrate. Our approach includes: (i) developing a bioconversion protocol for high-titre 2,3-BDO production from the yard waste hydrolysate; (ii) constructing a simultaneous saccharification and fermentation (SSF) process using an in-situ fibrous bed bioreactor (isFBB) technique to convert biomass-derived hemicellulose and glucose into 2,3-BDO, aiming to achieve a total yield of over 70%; (iii) upgrading 2,3-BDO into olefin intermediates and then into iso-alkane SAF precursors. The last part of the talk will introduce a recent project on co-hydrothermal liquefaction of microalgae biomass and food waste remaining solids. In this study, food waste hydrolysis was conducted using commercial enzymes, and nutrient-rich hydrolysate was used for the mixotrophic cultivation of microalgae *Euglena gracilis*. The proposed zero-waste production system illustrates promising application in green and sustainable organic waste valorization.

Keywords: Biofuels and chemicals; Microalgae, Polyurethane, Sustainable Aviation Fuel

SYNTHESIS OF SUPERABSORBENT HYDROGEL-BIOCHAR COMPOSITES AS NITROGENOUS CONTROLLED-RELEASE FERTILIZERS

Mohamad Izzat Arif Nordin^a, Dzureen Julaihi^a, Suk Fun Chin^b, Lin-Chi Wang^c,
Cindy Soo Yun Tan^{a,*},

^a*Faculty of Applied Sciences, Universiti Teknologi MARA, 94300 Kota Samarahan, Sarawak, Malaysia*

^b*Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak,
Malaysia*

^c*Department of Marine Environmental Engineering, National Kaohsiung University of Science and Technology,
142, Haijhuang Road, Nanzih District, Kaohsiung City, 81157, Taiwan*

*Corresponding author: cindytan@uitm.edu.my

Abstract

Traditional biochar-based fertilizers consisting of a mixture of biochar, chemical fertilizers and additives often exhibit rapid nutrient release, and low water-retention performance, thus limiting their effectiveness. Poor utilization efficiency of fertilizer coupled with freshwater resource scarcity have led to declining crop yields and environmental concerns. To address these issues, novel superabsorbent hydrogel-biochar composites based on potassium poly(acrylate-co-acrylamide) incorporated with urea (DHNBCUs) of varying ratio of biochar (BC), *N,N*-methylene bisacrylamide (MBA) crosslinker and poly(vinyl alcohol) (PVA) were synthesized via one-pot strategy. The FTIR and SEM results show the successful BC and urea encapsulation in the DHNBCUR1 and DHNBCUR7, with average urea loading efficiency (LE) of 12 -14% and encapsulation efficiency (EE) of 78 - 82%. The results showed that DHNBCUR1 with higher BC but lower MBA and PVA percentages exhibited superior water absorption (221.92 g/g) compared to DHNBCUR7 (209.13 g/g) in DI water, in which both DHNBCUs showed higher water absorption and swelling at pH 7 and 9 compared to pH 4. The swelling trend of DHNBCUs in different cationic salt solutions is $KCl > NaCl > MgCl_2 > CaCl_2 > FeCl_3$, with significantly lower water absorption ranging between 7.35 g/g and 31.34 g/g attributed to the charge to size ratio of the multivalent cations on the DHNBCU's charge density. Therefore, DHNBCUs have the potential to be widely applied in sustainable agriculture, owing to their ability to retain soil moisture, thus reducing irrigation water dependence, whilst improving fertilizer utilization efficiency of the conventional biochar-based fertilizers.

Keywords: Superabsorbent, hydrogel-biochar composites, water absorption, urea, controlled-release fertilizers

EFFECT OF ACID DOPANTS ON THE ANTIBACTERIAL PROPERTIES OF CARRAGEENAN/POLYANILINE FILMS

Sook-Wai Phang^{a*}, Wen-Qing Yang^a, Mei-Xin Koh^a, Ying-Chiang Low^a, Ishak Ahmad^b

^aFaculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology (TARUMT), 53300, Setapak, Kuala Lumpur, Malaysia.

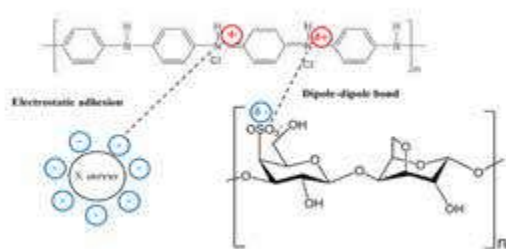
^bPolymer Research Centre (PORCE), Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600, Bangi, Selangor Darul Ehsan, Malaysia.

*Corresponding author: phangsw@taru.edu.my

Abstract

Synthetic and petrochemical based polymeric antibacterial materials are typically used as surface coatings and have since led to pollution. To overcome this problem, a biopolymer, κ -carrageenan (κ -CGN) was introduced as a matrix of the antibacterial film incorporating polyaniline (PAni) as the antibacterial agent. PAni was synthesised by chemical oxidative method with different acid dopants which are hydrochloric acid (HCl), sulphuric acid (H₂SO₄) and phosphoric acid (H₃PO₄) followed by characterisation of Fourier Transform Infrared Spectrophotometry (FTIR), Ultraviolet-Visible Spectrophotometry (UV-Vis), electrical conductivity and Thermogravimetric Analysis (TGA). Among all the doped PAni, PAni-H₂SO₄ showed the highest conductivity (29.33 S/cm) and decomposition temperature, T_d (536.74°C) compared to PAni-HCl (8.67 S/cm; T_d : 478.45°C) and PAni-H₃PO₄ (7.27 S/cm; T_d : 508.76°C). κ -CGN/PAni films were produced through ex-situ method and evaluated by FTIR, electrical conductivity, tensile test and TGA. κ -CGN/PAni films had successfully inhibited the growth of *S. aureus* (gram-positive bacteria) but not *P. aeruginosa* (gram-negative bacteria). The mechanism of the bacterial inhibition was suggested that the protonated PAni was electrostatically attracted to the anionic membrane of the bacteria and disrupted the membrane, leading to cell death. κ -CGN/PAni-HCl film had the best antibacterial performance as there was minimum PAni included in the film (10% wt PAni; inhibition%: 35.82%) compared to κ -CGN/PAni-H₂SO₄ film (20% wt PAni; inhibition%: 35.44%) and κ -CGN/PAni-H₃PO₄ film (30% wt PAni; inhibition%: 37.65%). It can be concluded that κ -CGN/PAni-HCl film was the best composite that possesses the highest antibacterial performance as well as good mechanical properties (tensile strength: 1.51MPa; elongation at break: 18.76%) by utilising minimum only 10% of PAni.

Keywords: acid dopants, antibacterial, carrageenan, conductivity, polyaniline.



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MODIFICATION OF STARCH BIO-NANOCOMPOSITE FOR ACTIVE AND INTELLIGENT FOOD PACKAGING

I. Ahmad^{*,1}, U. H. Abdullah¹, M.R. Chia¹, N. S. Mohd Razali² and S.W. Phang³

¹*Department of Chemical Sciences, Faculty of Science and Technology,
Universiti Kebangsaan Malaysia (UKM), 43600 Bangi, Selangor, Malaysia*

²*Department of Food Sciences, Faculty of Science and Technology,
Universiti Kebangsaan Malaysia (UKM), 43600 Bangi, Selangor, Malaysia*

³*Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University College, Kuala Lumpur 53300, Malaysia*

**Corresponding author: gading@ukm.edu.my*

Abstract

It is essential to produce eco-friendly bioplastics to meet the needs of the industrial sector and replace petroleum-based plastics, which have a severe environmental impact. The synergistic effects of both cellulose nanocrystals (CNC) and cinnamon oil (CO) were investigated in terms of the physical, mechanical, thermal, and antimicrobial properties of starch bio-nanocomposites. Antimicrobial analysis was performed using the disk diffusion method on four different types of microorganisms: *Bacillus cereus*, *Bacillus subtilis*, *Aspergillus niger*, and *Aspergillus brasiliensis*. The presence of cinnamon oil improved the antimicrobial activity and water barrier properties of the starch/cinnamon film. Additionally, it was found that the tensile strength was significantly improved with the addition of CNC. On the other hand, a food spoilage indicator for active and intelligent food packaging systems is crucial to address food wastage issues. Polyaniline (PANI) was incorporated into starch/PANI/CNC bio-nanocomposites to act as a food freshness indicator. The films were applied as real-time fish freshness indicators. The incorporation of CNC into starch/PANI films significantly improved the mechanical and thermal properties of the films. Starch films with 0.4 wt% PANI exhibited the optimal composition, with a radical scavenging capability of 15.18% and an excellent ammonia-sensing capability, where the low detection limit (LOD) was 145 ppm. Additionally, the inclusion of CNC did not significantly compromise the ammonia sensitivity (LOD: 52 ppm) of the film. Moreover, the in situ polymerization method enhanced the homogeneity of the starch bio-nanocomposite films, thus improving their mechanical strength. Most importantly, the film serves as a reliable fish freshness indicator and biodegrades by more than 70% within a month. Therefore, the starch/PANI/CNC biopolymer film has high potential for use as active and intelligent food packaging.

Keywords: *starch, cellulose nanocrystals (CNC), cinnamon oil (CO), polyaniline (PANI), empty fruit bunch (EFB)*

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VALORIZATION OF BLACK SOLDIER FLY (BSF) WASTE INTO CHITOSAN-BASED BIOPOLYMERS

Luísa M.D.R.S. Martins^{a,*}, Andreia Figueiras^a, Ana P.C. Ribeiro^a

^a Centro de Química Estrutural, Institute of Molecular Sciences, Chemical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Portugal.

*Corresponding author: luisammartins@tecnico.ulisboa.pt

Abstract

The insect industry has rapidly emerged as a key player in sustainable solutions for food, feed, agriculture, and biotechnology. This sector leverages insects' ability to efficiently convert organic waste into high-value products. *Hermetia illucens* (Black Soldier Fly, BSF), mealworms such as *Tenebrio molitor* (TM), and crickets like *Acheta domesticus* (AD), are among the most widely farmed species due to their rich protein content, rapid growth, and minimal environmental footprint. Of these, the Black Soldier Fly (BSF) stands out for its remarkable ability to reduce environmental pollution while generating protein, oil, and frass (insect manure) for various applications.

The conversion of insect biomass into valuable biopolymers presents an innovative and sustainable solution to pressing global challenges such as plastic waste and resource scarcity. The focus of this communication is on the extraction of chitin from BSF exuviae, and its conversion into chitosan and derivatives (Figure 1). Chitosan-based biopolymers have immense potential for use in a wide range of industries, including packaging, medicine, cosmetics and agriculture, where they could replace conventional plastic materials and synthetic polymers. The production of chitosan from insect-derived chitin presents significant advantages, such as reduced environmental impact, as these materials are biodegradable and have low toxicity. Moreover, the use of BSF exuviae helps address resource scarcity by providing a renewable, efficient, and scalable alternative to traditional biopolymer sources. This novel approach could substantially reduce the dependence on petrochemical-based products and contribute to the development of more sustainable practices in various sectors. This presentation will provide an in-depth exploration of the processes involved in BSF exuviae conversion, focusing on the chitin extraction and their deacetylation. Challenges and future directions in scaling up this process for industrial applications will be discussed, highlighting the importance of advancing research in this promising field of sustainable material production.

Keywords: insect waste valorization, chitin, chitosan, circular economy, sustainable chemistry



Figure 1. Repetitive units' representation of the chitin and chitosan biopolymers.

Acknowledgements



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ENHANCING THE PERFORMANCE OF POLY (LACTIC ACID)-CLAY NANOCOMPOSITES: MONTMORILLONITE MODIFICATION FOR SUSTAINABILITY

W.M.Z. Wan Yunus

National Defence University of Malaysia

Corresponding author: wanmdzin@upnm.edu.my

Abstract

Poly(lactic acid) (PLA) is an environmentally friendly polymer valued for its biodegradability and bio-based origin, making it a strong candidate for applications in packaging, biomedical devices, and structural materials. However, its intrinsic brittleness and limited thermal stability present challenges for high-performance applications. One effective strategy to enhance PLA's properties is the incorporation of montmorillonite (MMT) nanoclay, which can improve its mechanical strength, thermal stability, and barrier performance. However, achieving uniform dispersion and strong interfacial adhesion remains a key challenge, necessitating tailored modifications of MMT.

This presentation will describe our work on modifying MMT to improve its compatibility with PLA. The modification is achieved by intercalating large organic molecules into the MMT layers through ionic exchange. The modified MMT was characterized using various analytical techniques, including FTIR spectroscopy, elemental analysis, and thermogravimetry. Additionally, PLA-clay nanocomposites were prepared using melt blending or solvent casting, and impact of the MMT content on physical and mechanical of the final material properties was studied using various characterization methods.

This lecture will provide valuable insights for researchers, materials scientists, and industry professionals working on sustainable polymer composites, offering a deeper understanding of how functionalized MMT can enhance the performance of PLA-based materials.

Keywords: MMT modification, PLA-clay nanocomposites.

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AMINE-MODIFIED HYPERCROSSLINKED POLY(ACRYLONITRILE-CO-DIVINYLBENZENE-CO-VINYLBENZYL CHLORIDE) FOR ENHANCED ADSORPTION OF METRONIDAZOLE FROM AQUEOUS SOLUTION

Nur Afifah Nek Daud^a, Siti Nurul Ain Md Jamila,^{b*} Luqman Chuah Abdullah^c, Rusli Daik^d,
Nur Nida Syamimi Subria, Fatimah Lee Muhammad Hisyam Lee^a

^aChemistry Department, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

^b Centre for Foundation Studies in Science of Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

^cDepartment of Chemical and Environmental Engineering, Faculty of Engineering, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

^dDepartment of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.

*Corresponding author: ctnurulain@upm.edu.my

Abstract

The persistent presence of antibiotic residues, particularly metronidazole (MNZ), in aquatic environments poses a serious ecological and health concern. This study presents the synthesis and characterization of amine-functionalized hypercrosslinked terpolymers based on poly(acrylonitrile (AN)-co-divinylbenzene-80 (DVB80)-co-vinylbenzyl chloride (VBC)) for the adsorption of MNZ from aqueous solutions. The terpolymer was prepared via precipitation polymerization and subsequently hypercrosslinked using a Friedel–Crafts reaction with FeCl₃ as a catalyst. Amine functionalities were introduced by modifying the hypercrosslinked network with ethylenediamine (EDA) and diethylenetriamine (DETA) to enhance the availability of active adsorption sites. The synthesized materials were characterized using FTIR, SEM, BET, TGA, CHN elemental analysis, and point zero charge (pHPZC) determination. Adsorption experiments evaluated the influence of pH, initial MNZ concentration, contact time, and adsorbent dosage. The DETA-modified polymer showed superior amine density and slightly higher adsorption performance compared to the EDA-modified variant. These findings suggest that amine-modified hypercrosslinked polymers are promising candidates for efficient removal of antibiotic residues from contaminated water, contributing to sustainable water purification strategies [1].

Keywords: Metronidazole, hypercrosslinked polymer, amine modification, adsorption, wastewater treatment

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ACACIA GUM AS A NATURAL BIOPOLYMER ADDITIVE FOR IMPROVING HYDROPHILICITY AND CONDUCTIVITY OF ENDOCRINE DISRUPTING CHEMICALS (EDCS) ELECTROCHEMICAL BIOSENSORS

Sharina Abu Hanifah^{1*}, Anwarul Hidayah Zulkifli¹, Zalifah Mohd Kasim² & Masato Ikeda³

¹Department of Chemical Sciences, Faculty of Science and Technology, 43600 Universiti Kebangsaan Malaysia, Bangi, Selangor, Malaysia;

²Department of Food Science, Faculty of Science and Technology, 43600 Universiti Kebangsaan Malaysia, Bangi, Selangor, Malaysia;

³Department of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University, 1-1 Yanagido, Gifu 501-1193, Japan⁴

*Corresponding author: sharina@ukm.edu.my

Abstract

Numerous electrochemical biosensors have been developed over the years for detection of endocrine-disrupting chemicals (EDCs) such as Bisphenol A (BPA) and Diethylhexyl phthalate (DEHP), with a focus on achieving low limits of detection (LOD), high selectivity, sensitivity and stability^{1,2,3}. Despite these advancements, limited research has focused on the use of natural membrane additives like *Acacia gum* (AG), which offer potential benefits in enhancing biosensor conductivity, sensitivity, and selectivity. In this study, electrochemical biosensor membranes for BPA and DEHP detection were fabricated by blending methacrylic-acrylic monomers namely 2-hydroxyethyl methacrylate (HEMA) and n-butyl acrylate at 60°C for 30 minutes, incorporating 6% w/w AG and 0.05% w/w silver nanoparticles (AgNPs). The addition of AG reduced the membrane contact angle to below 50°, compared to 70° for membranes without AG, indicating increased hydrophilicity. FTIR revealed hydroxyl stretching and C–C bonding while O–H bending was attributed to the carboxylic acid groups in AG. The BPA electrochemical biosensor showed a wide linear detection range from 1×10^{-20} M to 1×10^{-10} M ($R^2 = 0.9504$), whereas the DEHP sensor exhibited a linear range from 1×10^{-14} M to 1×10^{-5} M ($R^2 = 0.9307$). Both sensors demonstrated strong selectivity for their respective targets and showed good agreement with HPLC results ($R^2 = 0.9801$) during validation using river water samples. In conclusion, the incorporation of *Acacia gum* as a natural biopolymer membrane additive not only contributed to the green design of the biosensor but also enhanced its performance by improving conductivity, hydrophilicity and selectivity, highlighting its potential in sustainable environmental monitoring.

Keywords: Endocrine disrupting chemicals (EDCs), *Acacia gum*, Bisphenol A (BPA), Diethylhexyl phthalate (DEHP), electrochemical biosensor

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BIOWASTE-DERIVED COMPOSITE MEMBRANES FOR OIL/WATER SEPARATION: MODIFICATION, FABRICATION, CHARACTERIZATION, AND PERFORMANCE EVALUATION

Rizafizah Othaman^{a,*}, Nurul Amni Abdullah^b, Siti Nurzubaida Shahdan^a, Nazwa Jon^b,
Diyana Kamarudin^a, Azizah Baharum^a.

^aUniversiti Kebangsaan Malaysia.

^bUniversiti Teknologi MARA.

*Corresponding author: rizafizah@ukm.edu.my

Abstract

Oil-in-water (O/W) emulsions in domestic and industrial effluents pose a significant treatment challenge due to their chemical stability, fine droplet size, and resistance to conventional separation techniques. This study presents the fabrication and evaluation of biodegradable composite microfiltration membranes based on a poly(L-lactic acid)/polycaprolactone (PLLA/PCL) matrix integrated with chemically modified eggshell particles (MESP). The MESP was synthesized via stearic acid esterification or modified with silane agents and incorporated into the polymer matrix to form asymmetric, porous membranes with micro/nano-hierarchical surface architecture. Membrane fabrication employed plate casting, non-solvent-induced phase separation (NIPS), glacial acetic acid surface treatment, and ambient drying. Comprehensive characterization was conducted to examine chemical structure (FTIR), crystallinity (XRD), morphology (SEM, AFM), mechanical properties, and wettability (WCA/OCA). The membranes were tested for separation performance using a surfactant-stabilized O/W emulsion. Results showed a gravity-driven oil removal efficiency averaging 78.9%, which increased to approximately 90% under 15-psi pressure-driven conditions using a dead-end stirred cell. The membranes were successfully regenerated via ethanol backwashing. This work demonstrates a green, cost-effective strategy for biowaste valorization and membrane fabrication, contributing to advanced oil/water separation technologies. The developed membranes offer high performance, sustainability, and reusability, making them promising candidates for wastewater treatment and environmental remediation applications.

Keywords: Chicken eggshell, modified composite membrane, O/W emulsion separation, wastewater treatment.

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SORPTION KINETICS AND DIFFUSION BEHAVIOUR OF POST-CHARACTERIZED, BIOMODIFIED WASTE PET (RIC-1) BOTTLES COMPOSITES

Onyinyechi Gift Aliene and Cyprian Yameso Abasi

Department of Chemical Sciences, Niger Delta University Wilberforce Island, Bayelsa State, Nigeria

Corresponding Author: onyinyechialiene@gmail.com

Abstract

This study dwelt on the preparation, characterization, and application of composites made from waste (PET) polyethylene terephthalate bottles with a resin identification code of 1 (RIC-1). These composites were prepared by melt mixing PET matrix with other fillers such as crab shell, clay, and chitin, resulting in binary or ternary composites. The physicochemical properties and characterization of the composites were analysed using techniques such as, porosity testing, pH point at zero charge, surface area and FTIR. The composites were thereafter applied for the remediation of iron (III) ions from aqueous solution in which the rate and diffusion dynamics are investigated with the pseudo-first order (PFO), pseudo-second order (PSO) and the Weber- Morris intraparticle diffusion models. The results showed that the pseudo-second order (PSO) kinetic model had a good correlation for all ternary composites, with R^2 values of 0.9977 for PET/CBS/CLAY and 0.9847 for PET/CHITIN/CLAY. The pseudo- first order (PFO) model also showed good correlation, with R^2 values of 0.9812 for PET/CHITIN/CLAY, 0.9276 for PET/CBS and 0.9207 for PET/CHITIN. These results suggest that PSO was more prevalent, and therefore infer that chemisorption was the dominant mechanism for adsorption in these composites. Webber-Morris intraparticle diffusion model applied to data gave a multi-linear correlation of the adsorption of Fe (III) ions on the binary and ternary composites as well as the single materials. However, R^2 values of crab shell, clay, chitin, PET/CLAY, PET/CBS, PET/CHITIN, and PET/CBS/CLAY, were 0.9509, 0.9737, 0.9492, 0.9366, 0.9063, 0.9317, and 0.9169 respectively. The high R^2 values of the rate models shows a positive adsorbent behaviour of the composites.

Keywords: Sorption, kinetics, diffusion, composites, bio-modified, waste PET bottles.

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DIETARY POLY- β -HYDROXYBUTYRATE (PHB) GRANULES IMPROVED GROWTH AND RESISTANCE AGAINST ACUTE HEPATOPANCREATIC NECROSIS DISEASE PATHOGENS IN WHITE-LEG SHRIMP (*Litopenaeus vannamei*)

Nur Liyana Ismail^{a*}, Siti Amira Mat Hussin^a, Mong Mei Ling^b, Sara Shahrudin^a,
Navin Sharma Karam Chand^a, Jofry Othman^a & Kumar Sudesh^b

^aPETRONAS Research Sdn. Bhd., Lot 3288 and 3289, Off Jalan Ayer Itam, Kawasan Institusi Bangi, 43000 Kajang, Selangor Darul Ehsan, Malaysia

^bEcobiomaterial Research Laboratory, School of Biological Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia

*Corresponding author: nurliyana.ismail@petronas.com

Abstract

Aquaculture has become even more important as a source of fish for human consumption. The Pacific white shrimp, also known as the white leg shrimp (*Litopenaeus vannamei*) is a highly valuable aquaculture export, commanding a significant portion of the market share. A developing bacterial disease, acute hepatopancreatic necrosis disease (AHPND), has had a devastating impact on the global shrimp industry over the last ten years. Short-chain fatty acids (SCFAs) have been proposed as an alternative to antibiotics for controlling diseases in aquaculture. However, SCFAs have properties such as corrosiveness, a strong odour, and high-water solubility. These characteristics make their absorption by aquatic animals inefficient and unsuitable for direct application in aquaculture.^{1,2} Poly- β -hydroxybutyrate (PHB) is a storage compound for energy and carbon that is produced by various microorganisms. PHB is a non-toxic and biodegradable polymer and has the potential for use as a feed additive in aquaculture. It is hypothesized that when PHB is supplemented through feed, it will be biologically broken down into SCFA β -hydroxybutyric acid or PHB oligomers within the gastrointestinal tract of aquatic animals. This process results in a slightly lower intestinal pH, thus enhancing the activity of beneficial gut flora.³ This study investigated the effects of supplementing shrimp diets with varying molecular weights of PHB granules at concentrations of 0.05% and 0.10%. Results demonstrated that dietary inclusion of PHB significantly enhanced shrimp growth performance and increased resistance to AHPND. The observed improvements were linked to a reduction in bacterial counts and minimized tissue damage in the hepatopancreas. These findings highlight the potential of PHB as a functional feed additive to improve shrimp health and productivity. The incorporation of PHB into shrimp diets offers a promising strategy for developing high-quality aquaculture feeds, ultimately contributing to increased shrimp production yields.

Keywords: Poly- β -hydroxybutyrate (PHB), *Litopenaeus vannamei*, Short-chain fatty acids (SCFA), Growth performance, AHPND

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DIRECT EXTRACTION OF NATURAL CANNABINOIDS FROM HEMP LEAVES AND SUSTAINABLE PLGA NANOCARRIERS FOR ENHANCED CBD DELIVERY

Sumontha Ramangkoon^{1,2}, Brian J. Tighe³, Matthew J. Derry³, Jutamas Jiaranaikulwanitch⁴, Puttinan Meepowpan^{1,2}, Donraporn Daranarong^{2,5}, Chanakarn Srimuang⁶, Paul D. Topham³, Winita Punyodom^{1,2,*}

¹ Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

² Bioplastic Production Laboratory for Medical Application, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

³ Aston Institute for Membrane Excellence, College of Engineering and Physical Sciences, Aston University, Birmingham, B4 7ET, United Kingdom

⁴ Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai 50200, Thailand

⁵ Multidisciplinary Research Institute, Chiang Mai University, Chiang Mai 50200, Thailand

⁶ Chanaka Dhibesra Damri Royal Project Agricultural Research and Development Center, Chiang Mai 50100, Thailand

*Corresponding author: winitacmu@gmail.com

Abstract

Cannabis sativa L. (hemp) is a sustainable source of cannabinoids, including non-psychoactive cannabidiol (CBD) and psychoactive tetrahydrocannabinol (THC), both of which exhibit significant pharmacological properties such as neuroprotection, antioxidant activity, and anti-inflammation. However, cannabinoid-based therapeutics face challenges related to instability, poor water solubility, and low bioavailability, limiting their clinical efficacy. A significant research gap exists in the development of sustainable drug delivery technologies derived from hemp leaves. This study reports the extraction of cannabinoids with high antioxidant and CBD content directly from hemp leaves in a straightforward, simple process. The extract was then loaded within bio-based and biodegradable polymer nanoparticles using a single emulsion evaporation method, targeting nanoparticle sizes below 200 nm to enhance drug delivery efficiency. Process parameters have been systematically studied to optimize nanoparticle characteristics. The resulting nanoparticles exhibited reproducible properties, acceptable encapsulation efficiency, and storage stability for at least six months. Drug release studies indicated a diffusion-based mechanism, supporting their potential for controlled drug delivery. These findings highlight the feasibility of utilizing sustainable hemp leaf-derived cannabinoids in PLGA-based nanocarriers, providing an eco-friendly and scalable approach for enhancing cannabinoid bioavailability. This work contributes to the development of sustainable drug delivery systems and adds value to hemp-derived bioactive compounds for therapeutic applications.

Keywords

Hemp leaves, Cannabinoids, Biodegradable polymer, Nanoparticles, Encapsulation, Drug delivery

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REPURPOSED DIELECTRIC-POLED FUNCTIONAL POLYMERS FOR SUPERCAPACITOR: A NOVEL STRATEGY FOR ENERGY AND ENVIRONMENTAL REMEDIATION

Priyanka Bhardwaj^a, Mamta Latwal^a, Tridib Kumar Sinha^a

^aUniversity of petroleum and energy studies - Dehradun (India)

*Corresponding author: PRIYANKA.105139@stu.upes.ac.in

Abstract

The global energy model is escalating the demand of alternate cleaner and renewable energy instead of the traditional practices considering the future exhaustion of fossil fuel and related global warming issues. This transformation needs a low-cost, reliable, efficient, lightweight, flexible energy storage device such as Supercapacitors to realize a sustainable and continuous power supply. The fundamental constituents of a flexible supercapacitor include flexible electrodes, an electrolyte medium, and a flexible dielectric separator. This research focuses on the development of solid-state supercapacitors using both dielectric polymer and bio-polymer wastes as a sustainable resource to create a flexible device. For instance, polyurethane (PU), which contributes almost 45% of synthetic polymer waste, not only possess polarizable functional groups (e.g., -O-C(=O)-NH) but also various tailorable properties, e.g., adorable tensile property, elasticity, flexibility, processability (being a thermoplastic elastomer), and compatibility to broad range of fillers. In this study, composites of PU with dielectric bio-polymers such as keratin, protein found in nails, hair and skin contains several functional groups such as -NH₂, -COOH, -S-S, incorporated with conductive filler i.e. Graphite was grown under an applied electric field to produce flexible polarized films exhibiting enhanced supercapacitor performance. A cellulose-based hydrogel was also developed to be used as separator and supporting medium for ionic transportation to realize a solid-state supercapacitor. The resulting flexible supercapacitor exhibited a high specific capacitance of 19.36 mF/cm² at a scan rate of 5mV/s and a maximum energy density of 1.72 mWh/cm² at an operating voltage of 0.8 V. This work introduces a novel pathway for the utilization of dielectric polymer waste in energy storage devices, paving the way for applications in automation, wearable electronics, and beyond.

Keywords: Dielectric, Biopolymer, Supercapacitor

BIOACTIVE WOUND DRESSING BASED ON CHITOSAN–GELATIN NANOFIBERS LOADED WITH CURCUMIN/CHRYSLIN-FUNCTIONALIZED METAL–ORGANIC FRAMEWORKS

Yoon Yee Then^{a,*}, Soo Ghee Yeoh^b, Norizah Abdul Rahman^c, Yun Khoon Liew^d, Wei Meng Lim^e, May Lee Low^f, Lai Chun Wong^a

^aDepartment of Pharmaceutical Chemistry, School of Pharmacy, IMU University, Malaysia.

^bSchool of Postgraduate Studies, IMU University, Malaysia.

^cDepartment of Chemistry, Faculty of Science, Universiti Putra Malaysia, Malaysia.

^dDepartment of Life Sciences, School of Pharmacy, IMU University, Malaysia.

^eSchool of Pharmacy, Monash University Malaysia, Malaysia.

^fSchool of Pharmaceutical Sciences, UCSI University, Malaysia.

*Corresponding author: thenyoonyee@imu.edu.my

Abstract

Effective wound management requires materials that not only protect the wound site but also actively promote healing and prevent infection. In this study, a bioactive wound dressing was developed using chitosan–gelatin (CS–Gel) electrospun nanofibers incorporated with curcumin/chrysin-functionalized metal–organic frameworks (MOFs). Curcumin (Cur) and chrysin (Chr), both natural flavonoids with proven antioxidant, anti-inflammatory, and antimicrobial properties, were utilized to functionalize the MOFs, enhancing their stability and controlled release potential within the nanofiber matrix. The hybrid nanofibers were fabricated via electrospinning, resulting in a highly porous, biocompatible scaffold suitable for wound applications. Physicochemical analyses confirmed the successful incorporation of the Cur/Chr-functionalized MOFs into the CS–Gel matrix, with improved moisture retention, and structural integrity. *In vitro* assays demonstrated strong antibacterial activity against both *Staphylococcus aureus* and *Pseudomonas aeruginosa*, while cytocompatibility tests showed enhanced keratinocyte proliferation. Furthermore, the sustained release of curcumin and chrysin from the nanofibers contributed to prolonged therapeutic action. These findings suggest that the Cur/Chr-functionalized MOF-loaded CS–Gel nanofiber dressing holds strong potential as an advanced wound healing material, offering both structural support and bioactive functionality for infection control and tissue regeneration.

Keywords: Chitosan, gelatin, curcumin, chrysin, metal-organic frameworks

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ANALYTICAL CHEMISTRY IN COURTS OF LAW

D Brynn Hibbert^{a*}

^a School of Chemistry, UNSW Sydney, Sydney NSW 2052 Australia.

b.hibbert@unsw.edu.au

Abstract

Although the law professes to demand surety in its determinations – ‘beyond reasonable doubt’, etc. courts are remarkably ignorant of how science works to provide that surety and have a deep distrust of statistics.

The concept of ‘reliability’ of expert evidence is a hot topic in forensic science [1]. Although high profile cases have often been concerned with soft sciences, such as shoe prints, bite marks, or identification of recorded voices, DNA analysis still remains in contention for the most probed analytical technique, and the identification of drugs also poses problems. Accreditation, usually to ISO/IEC 17025:2017[2] is key to establishing the authority of a laboratory to identify, for example, a white powder found in possession of a suspect. Most official forensic laboratories (police, state, sports organizations) are obliged to be accredited, but when amateur scientists (forensic amateurs, often from good universities) become involved things can be very tricky. In a case during COVID [3], lead isotope analysis of bullets in a body that matched those in a box of bullets owned by a friend of the accused looked very sound until it was pointed out there was no validation. The prosecution case also fell foul of the likelihood of another box of bullets being sold at the same time.

In a more recent case, a court had to evaluate the difference between a presumptive and a confirmatory test. Benzyl cyanide had been intercepted at an Australian border and tested with hand-held infrared and Raman devices. The spectra were excellent, but the court ruled that without a sample being confirmed in a laboratory the match could not be sustained.

Chemists should engage with the law. It is difficult, courts really do not speak the same language, but lawyers and judges are intelligent and can be taught – by the right people.

Keywords: forensic science, analytical chemistry, isotope analysis, infrared, Raman

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USE OF UNCONVENTIONAL SOLVENTS, GREENER APPROACHES TO SAMPLE PREPARATION IN ENVIRONMENTAL ANALYSIS AND CURRENT CHALLENGES

Slavica Ražić^{a,*}, Jelena Arsenijević^a, Tatjana Trtić-Petrović^b

^aFaculty of Pharmacy, University of Belgrade

^bVinča Institute of Nuclear Sciences, University of Belgrade

*Corresponding author: slavica.razic@pharmacy.bg.ac.rs

Abstract

The development of a new generation of environmentally friendly solvents is based on *a priori* knowledge and experience. The achievements of the last decade will provide new perspectives and ideas for solving problems with different environmental samples. Sample preparation is still considered a bottleneck of the entire analytical process and cannot be completely avoided. The second environmentally friendly option after the “no solvent” scenario is the use of water, the safest and most abundant molecule on the earth’s surface, which is ecologically safe and non-toxic. By carefully tuning temperature and pressure, its physicochemical properties change significantly, increasing its solvent potential and selectivity for extracting compounds in a wide polarity range. Supercritical fluids (SCF) and especially CO₂ are attractive unconventional solvents with excellent solvent properties and an alternative to replace hazardous organic solvents. Due to their lower cost, reusability and environmental friendliness, both water and carbon dioxide are a good choice for sample preparation of environmental matrices. Conventional solvents are still used in laboratory practice but are increasingly being replaced by environmentally friendly solvents. Remarkable progress has been made in the field of ionic liquids (ILs) and deep eutectic solvents (DESS), also known as designer solvents. The numerous applications of ILs, DESS, SCW and SCFs as greener alternatives to conventional organic solvents in various environmental matrices offer a variety of solutions while challenging numerous environmental problems. One of the biggest challenges for the future will be to find a compromise between the increasing demands on the quality of the results (accuracy, LOD, reproducibility) and the improvement of environmental friendliness. There is no doubt that by implementing the principles of green (analytical) chemistry, we have paved the way for sustainable chemistry and the future in general.^{1,2}

Keywords: green chemistry, ionic liquids (IL), deep eutectic solvents (DES), supercritical fluids (SCF), subcritical water (SCW)

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PLASMONIC SINGLE-MOLECULE AFFINITY DETECTION AT 10 ZEPTOMOLAR

Luisa Torsi

Dipartimento di Chimica – Università degli studi di Bari

**Corresponding author: luisa.torsi@uniba.it*

Abstract

DNA can be amplified efficiently through replication, enabling the detection of a single target copy. In contrast, achieving similar sensitivity for protein detection in immunoassays remains an unresolved challenge. Surface plasmon resonance (SPR) is a well-established method for performing assays, typically achieving detection thresholds at concentrations around 10^{-9} molar.

This study demonstrates plasmonic single-molecule assays for both proteins and DNA, reaching detection limits (LODs) as low as 10^{-20} molar (1 ± 1 molecule in 0.1 mL) within 1 hour, even in complex samples like human serum. This represents an extraordinary eleven-order-of-magnitude improvement over standard SPR detection limits.

The enhanced sensitivity is achieved using a millimeter-scale surface coated with a physisorbed biolayer. This biolayer, containing trillions of recognition elements such as antibodies or protein-probe complexes, undergoes pH-conditioning in either acidic or alkaline environments. Investigations using potentiometric and surface-probing imaging reveal a previously unrecognized amplification mechanism responsible for this exceptional performance.

The findings suggest that pH-conditioning induces a metastable state in the biolayer, which facilitates a self-propagating aggregation of partially misfolded proteins upon single-affinity binding. This aggregation results in significant electrostatic rearrangement, corresponding to a displacement of approximately $1.5e$ per 10^2 recognition elements.

These insights pave the way for ultrasensitive SPR-based biosensing technologies capable of operating at the physical limits of detection. Such advancements hold great promise for the development of next-generation plasmonic systems tailored for point-of-care diagnostics.

Keywords: plasmonic sensors; single-molecule sensing; single-molecule with a large transistor (SiMoT); surface probing techniques; surface-plasmon-resonance.

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MULTIDIMENSIONAL GAS CHROMATOGRAPHY-MASS SPECTROMETRY FOR THE ELUCIDATION OF COMBUSTION RELATED ORGANIC AIR POLLUTANTS

Patricia Forbes^{a*} and Genna-Leigh Geldenhuys^{a,b}

^a*Department of Chemistry, University of Pretoria, Pretoria, South Africa.*

^b*Marine and Coastal Ecosystems Centre, Cyprus Marine and Maritime Institute, Larnaca, Cyprus.*

**Corresponding author: patricia.forbes@up.ac.za*

Abstract

Air quality has a direct impact on human health, with air pollution being the second largest mortality risk factor in 2021 accounting for 8.1 million deaths worldwide [1]. Combustion is a known source of organic air pollutants, including polycyclic aromatic hydrocarbons (PAHs), many of which may negatively impact human health with particular reference to respiratory disease. Combustion emission sources include biomass burning and diesel engine combustion. A robust analytical methodology is required to determine the impact of these activities on air quality. Multidimensional gas chromatography-mass spectrometry (GCxGC-MS) is an indispensable tool in this regard, as the enhanced separation which it provides enables correct peak identification and quantification. The results of studies are presented which aimed to assess potential improvements in air quality upon implementation of combustion-related interventions. The first involved replacement of diesel with biodiesel in fueling vehicles, which was tested under controlled laboratory conditions and then in an underground platinum mine. Sampling of gaseous semi-volatile organic compound (SVOC) emissions onto portable multichannel polydimethylsiloxane (PDMS) traps was conducted, followed by thermal desorption (TD)-GCxGC-MS analysis. A reduction in total gas phase PAH concentrations from 34 to 9 $\mu\text{g m}^{-3}$ was achieved when substituting diesel with biodiesel under high idle heavy-duty engine conditions in the underground mine [2]. Another study focused on the removal of unwanted sugar cane biomass prior to harvest, which is currently achieved by combustion in South Africa. Simultaneous sampling of gas and particle bound SVOCs before and after burn events was conducted using portable PDMS trap-based denuders. Total PAH concentrations (gas + particle phase) ranged from 0.05 to 9.85 $\mu\text{g m}^{-3}$ per burn event [3]. Over 85% of all PAHs were found to exist in the gas phase, causing the majority of variance between the burn sites which could be linked to the crop variety. The results of these studies highlight the importance of the comprehensive analysis of organic pollutant emissions in order to assess improvement interventions and inform effective management, thereby minimizing environmental and human health impacts.

Keywords: multidimensional gas chromatography-mass spectrometry, thermal desorption, semi-volatile organic compound, polycyclic aromatic hydrocarbon, air pollution

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ACCELERATED REACTIONS IN MICRODROPLETS: MECHANISMS AND APPLICATIONS IN ORGANIC SYNTHESIS AND DRUG DISCOVERY

Cooks, R. Graham, Morato, N. M.
 Purdue University, W. Lafayette, Indiana, USA
 *Corresponding author: cooks@purdue.edu

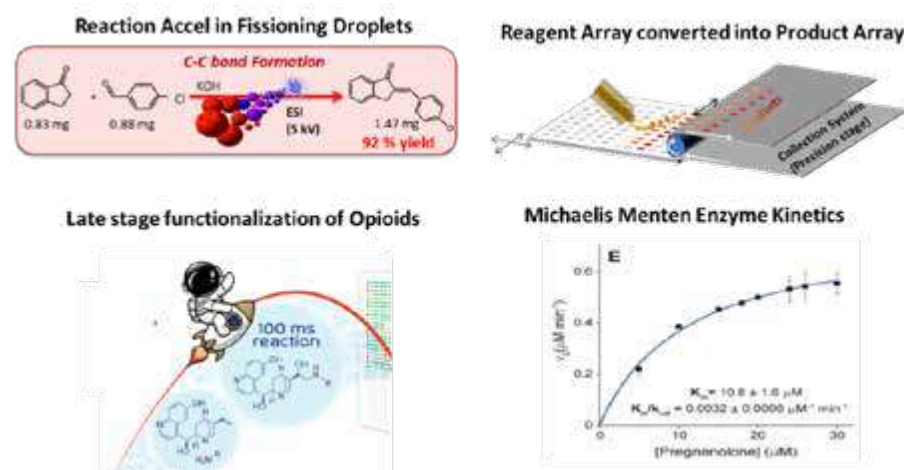
Abstract

The phenomenon of **accelerated chemical reactions in microdroplets** (rate constants increased by up to a million-fold relative to bulk) is introduced and its history is sketched.[1] The key role of the air/solution interface is demonstrated and the range of accessible chemistry is shown.

The aim is to understand and utilize accelerated microdroplet chemistry.

Microdroplets are generated by spray methods, including desorption electrospray ionization.

The factors that drive acceleration are **partial solvation** and **high interfacial electric fields**. Acceleration occurs in organic as well as aqueous microdroplets where **super-acid** and super-base species drive these reactions.[2] Most important is the water radical cation H_2O^+ and its monohydrate ($\text{H}_2\text{O}^+\cdot\text{H}_2\text{O}$, especially the isomer $\text{HO}\cdots\text{H}_3\text{O}^+$) which drives redox as well as acid/base chemistry. Redox reactions on sulfones, phosphonates and ketones will be noted as will condensation reactions leading to biopolymers (e.g. peptides) and to heterocyclic systems. A role for these catalyst free reactions in prebiotic chemistry is argued. Scale up of accelerated reactions (to g/hr levels) will be shown. Accelerated reactions are also performed on reaction mixtures in array format using desorption electrospray ionization (DESI) mass spectrometry.[3] This allows high throughput (**HT**) **reaction screening** (analysis of 6,144 reaction mixtures per hour, 5 ng scale). This new HT system is used for **small scale synthesis**, simply by collecting the **sprayed droplets on a 2nd array**. Further extension of the technology is shown in its **use in bioassays** and as an approach to early stage **drug discovery**. [3,4]



Keywords: Chemical synthesis; mass spectrometry; interfacial reactions; reactive intermediates;

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COMBINED ANALYTICAL METHODES FOR THE STRUCTURAL CHARACTERIZATION OF ISOMERS MIXTURES

Aura TINTARU

Aix-Marseille University, CNRS, CINaM – UMR7325, Marseille - FRANCE.

**Corresponding author: aura.tintaru@univ-amu.fr*

Abstract

For several years now, essential oils (EOs) have been attracting growing interest from the public, who invest lavishly in skincare products with exceptional properties. Obtained from aromatic, perfumed and medicinal plants, these complex mixtures made up of dozens of molecules offer a wide range of applications in cosmetics, food processing, aromatherapy, perfumery, medicine, etc. [1, 2] To explore at maximum their beneficial properties, we need to know their chemical, physico-chemical and biological characteristics, and identify the hazards associated with the production, marketing and use of these high added-value products. It has become essential to have a reliable and rigorous analytical sequence capable of gathering the new demands of consumers in terms of quality and safety.

Therefore, for reliable characterization of natural mixtures, each of the constituent products must be described in terms of its concentration, structure and, where appropriate, stereochemistry. Moreover, enantiomer-specific identification of chiral molecules in natural extracts is a challenging task, as many routine analytical techniques fail to provide selectivity in multi-component mixtures and/or lack sensitivity for dilute samples. Hence, the most challenging issue remains isomers identification and characterization. To do this, combined analytical strategies are used to provide the most detailed possible composition of each studied sample. Today, in addition to the analytical methods traditionally used (GC-MS, LC-MS, SPE, NMR), more modern techniques are being used (ESI-MS, tandem mass spectrometry, ion mobility coupled with mass spectrometry).

In this context, through some practical examples this presentation will illustrate alternative approaches, based on the combination of NMR, ion mobility-mass spectrometry (IM-MS) and quantum chemistry (QM), for the direct isomers' differentiation in crude essential oils and other complex samples. [3, 4]

Keywords: Essential oils, isomers, Mass Spectrometry, Ion mobility, NMR

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ADVANCES IN REFERENCE MATERIAL DEVELOPMENT FOR FOOD SAFETY AND NUTRITION ANALYSIS IN CHINA

^{1*}Hongmei LI^a; ²Sheng WANG^b; ³Tianji ZHANG^b; ⁴Ying KAN^b; ⁵Dan SONG^b

^aBeijing University of Chemical Technology

^bNational Institute of Metrology, China,

*Corresponding author: lihm@buct.edu.cn

Abstract

Reference Materials (RMs) are essential tools for ensuring the accuracy, comparability, and traceability of food safety testing results. Within the Global Measurement System (GMS), RMs establish metrological traceability to national standards and the International System of Units (SI), providing critical support for food safety and Nutrition analysis. In recent years, China has made significant progress in developing RMs for food nutrition and health, establishing a systematic RM framework. However, challenges persist, including insufficient coverage of complex matrices, limited detection capabilities for emerging hazardous substances, and gaps in RM development for specific Nutrition components, necessitating further technological innovation and system optimization. The National Institute of Metrology (NIM), China, has achieved notable advancements in high-precision detection technologies. Innovations in multi-parameter measurement techniques, including bidirectional salt precipitation, dual purification, and emulsification-demulsification, have improved sample preparation efficiency for high-fat and high-starch foods. Additionally, stable isotope labeling has enabled the synthesis of 65 isotope-labeled RMs across 13 categories of pesticides and illegal additives, providing precise benchmarks for trace-level contaminant quantification. The integration of database-driven intelligent RM development systems has further enhanced selection efficiency and testing accuracy. As of 2024, China has developed over 2,700 food-related RMs, covering key matrices such as grains, dairy, and seafood, and addressing contaminants like pesticide residues and toxins. However, gaps remain in specialized foods (e.g., fermented and functional foods), emerging pollutants (e.g., microplastics), and complex vitamins and Nutrition fortifiers. Future RM development will focus on detecting novel Nutrition and bioactive components, improving sensitivity for hazardous substance analysis, and integrating high-resolution mass spectrometry (HRMS) and nuclear magnetic resonance (NMR). Promoting international benchmarking and standardization will strengthen China's technical influence in global food safety. Through interdisciplinary collaboration and international cooperation, China aims to enhance food safety testing capabilities and contribute to global food quality control and regulatory frameworks.

Keywords: Reference Materials (RMs), Food Safety, Complex Matrices, Isotope Labeling, High-Resolution Mass Spectrometry

SHAPING THE FUTURE OF ANALYTICAL SCIENCE: PRECISION, SPEED, AND SUSTAINABILITY

Chee-Sian GAN ^{a*}

^a *Agilent Technologies Inc.*

* *Corresponding author: chee-sian.gan@agilent.com*

Abstract

Analytical science is undergoing a profound transformation, driven by the convergence of advanced instrumentation, digital innovation, and interdisciplinary collaboration. As global challenges in healthcare, environmental sustainability, and materials science intensify, the demand for faster, more precise, and more accessible analytical solutions continues to grow. **Agilent Technologies** is at the forefront of this evolution, delivering state-of-the-art tools that empower scientists to generate high-quality data and actionable insights.

Central to Agilent's contribution is the **InfinityLab LC Series**, including the Infinity III HPLC systems, which offer exceptional performance, reliability, and flexibility for a wide range of applications. These systems are designed to support high-throughput workflows with enhanced sensitivity and reproducibility, making them indispensable in pharmaceutical development, food safety, and environmental testing. When integrated with **Agilent's OpenLab** software and cloud-based platforms, these instruments enable seamless data acquisition, analysis, and compliance management.

Agilent's broader portfolio, including **LC/MS, GC/MS, ICP/MS**, and molecular spectroscopy, continues to evolve with Automation and Intelligence capabilities that streamline complex analyses and reduce time-to-result. These systems are instrumental in addressing emerging environmental concerns such as **per- and polyfluoroalkyl substances (PFAS)**^{1,2}. Agilent's solutions provide the sensitivity and selectivity required for trace-level PFAS detection in complex matrices, supporting regulatory compliance and environmental safety initiatives worldwide.

Sustainability is a guiding principle in Agilent's innovation strategy, with a focus on reducing solvent use, energy consumption, and laboratory waste. By combining technological excellence with a commitment to sustainability and accessibility, Agilent Technologies is helping to shape a future where analytical science is more agile, inclusive, and impactful than ever before.

Keywords: Sustainability, LC/MS, GC/MS, ICP/MS, HPLC, PFAS, Automation

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RECENT ADVANCES IN THE DEVELOPMENT AND APPLICATION OF CHEMICAL SENSORS BASED ON MOLECULARLY IMPRINTED POLYMERS

Amine A^{a*}

^a Faculty of Sciences and Techniques, Hassan II University of Casablanca (Morocco)

*Corresponding author: aziz.amine@fstm.ac.ma; azizamine@yahoo.fr

Abstract

Molecularly imprinted polymers (MIPs) are widely recognized for their exceptional selectivity, stability, and cost-effectiveness, making them valuable in biosensors, separation, and drug delivery applications. However, certain drawbacks limit their performance and versatility, including:

1. Incomplete and Time-Consuming Template Removal: Residual template molecules may remain trapped within the polymer matrix.
2. Non-Specific Adsorption [1]: MIPs can exhibit non-specific interactions, particularly in complex samples (e.g., biological fluids or environmental matrices), due to hydrophobic or electrostatic characteristics.
3. Time-Intensive Synthesis: The multi-step process of polymerization, cross-linking, and template removal is often labor-intensive and time-consuming.
4. Scalability Challenges: Producing MIPs in large quantities with consistent quality remains a significant hurdle.

To address these limitations, our research focuses on advancing polymer chemistry, nanotechnology, and green synthesis methods. Rapid and complete template removal has been achieved by employing optimized reagents. Post-modification of synthesized MIPs with hydrophobic aliphatic chains effectively suppresses non-specific adsorption [1]. Additionally, using ultrasonic probes, UV lamps, and visible laser excitation has significantly reduced MIP synthesis times from several hours to just a few minutes. A high-throughput and cost-effective approach for scalable MIP production has also been developed using lab-on-paper devices integrated with MIPs.

Furthermore, this presentation will explore recent advances in integrating MIPs with nano-catalysts to create innovative biomimetic sensors [2]. Key challenges and future perspectives for this field will also be outlined and discussed [3].

Keywords: chemical sensors; Molecularly imprinted polymers; nanotechnology; Non-Specific Adsorption; nano-catalysts

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HOW EFFICIENT CAN BE DIGESTION SYSTEMS USING DILUTED ACIDS FOR THE DETERMINATION OF REE AND TOXIC ELEMENTS IN EDIBLE INSECTS BY ICP-MS?

Érico Marlon de Moraes Flores^{a,*}

^a*Federal University of Santa Maria - UFSM.*

^{*}*Corresponding author: ericommf@gmail.com*

Abstract

Nowadays, food production has become a challenge, mainly due to demographic expansion and edible insects have many nutritional, breeding, and environmental benefits, providing an alternative to the growing food demand. Insects can be consumed at various stages of their life cycle, including larvae, eggs, pupae, and adults and they present higher levels of proteins, lipids, vitamins, and minerals (such as Ca, Fe, K, Mg, and Se), when compared to traditional protein sources. Thus, it becomes necessary to ensure that insects can be safely consumed, and quality control is of utmost importance, including the determination of toxic elements as Cd and Pb as well as emerging contaminants, such as rare earth elements (REE). There are few reports on sample preparation of edible insects, as wet digestion using microwave or conventional heating. However, these methods use relatively low sample masses (up to 300 mg), very long reaction times (up to 12 h for conventional acid digestion), and concentrated acids, resulting in final solutions with high carbon and acid content, which can cause interferences in ICP-MS analysis. In this lecture recent advances for the digestion of insects will be presented with a main focus on the use of high efficiency methods using UV radiation coupled to microwaves and special combustion methods combined to a microwave field as well as the use of diluted reagents assuring a full suitability for ICP-MS analysis virtually free of interferences. Applications for several species of edible insects will be presented for the determination of toxic elements as well as REE in these matrices in relatively short digestion time.

Keywords: edible insects, sample preparation, ICP-MS, microwave induced combustion, UV-digestion

THERMAL MANAGEMENT OF METAL HYDRIDE REACTOR

Ying Xu^{a*}, Mohammed Farid^b, Murray McCurdy^c, Fei Yang^a

^a Waikato Centre for Advanced Materials and Manufacturing, School of Engineering, University of Waikato,
Hamilton 3240, New Zealand.

^b Phase Foam Limited, New Zealand

^c Isotope Centre, GNS Science, PO Box 30368, Lower Hutt 5010, New Zealand

*Corresponding author: sherry.xu@waikato.ac.nz

Abstract

To meet the massive increase in energy demand, extensive research has been conducted on clean and sustainable energy storage over the past few decades.¹ Hydrogen energy is considered as one of the most promising future energy sources due to its high-energy density and renewability, but it requires storage. Storing hydrogen using metal hydride (MH) offers several advantages, including stability, safety compactness and reversibility of the hydrogen absorption and desorption process.²

Thermal management of metal hydride hydrogen storage systems is critically important since the reaction between the metal and hydrogen is highly exothermic.³ We are aiming to develop thermal storage systems based on composites phase change materials (CPCM), which are able to absorb the heat generated during adsorption and release it during desorption; otherwise, the energy storage efficiency will be poor.

Lightweight, shape-stable CPCM are prepared by loading the selected organic PCM into expanded graphite (EG) and hydrophobic silica aerogel (Si_{agl}). The chemical structure, microstructure, thermal properties and leakage of CPCM are investigated and will be discussed. An electric heater with varying power will be used to simulate the heat generated from the reaction between hydrogen and the metal, which follow first order kinetics.

Keywords: Thermal management, Composite Phase Change Materials, Thermal properties, Metal hydride reactor

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RADIAL FLOW STREAM SPLITTING FOR IMPROVED SEPARATION AND WORKFLOW FOR A GREENER APPROACH TO ASTAXANTHIN ANALYSIS

Karin Luize Mazur^{ab}, Xavier Anthony Conlan^b, Ross Andrew Shalliker^c, Luis Afonso^b

^a *ARC Industrial Transformation Training Centre for Green Chemistry in Manufacturing.*

^b *Centre for Sustainable Bioproducts (CSB), School of Life and Environmental Sciences, Deakin University, 75 Pigdons Road, Waurin Ponds, Victoria 3216, Australia.*

^c *Australian Centre for Research on Separation Science (ACROSS), School of Science and Health, Western Sydney University, Parramatta, NSW 2150, Australia*

**Corresponding author: k.mazur@deakin.edu.au*

Abstract

A newly developed radial flow splitting (RFS) column was used for high-throughput RP-HPLC analysis of astaxanthin (AST) and its esters in fish feed. AST, a potent antioxidant and carotenoid pigment, is crucial in aquaculture for enhancing fish health, immune response, and pigmentation [1–3]. As an expensive additive, its precise analysis in fish feed is essential for quality control, ensuring optimal nutrition, and supporting economic returns for producers. A chromatography column fitted with the RFS end fitting function was designed to offer higher speed, higher efficiency, and improved separation performance metrics in general compared to conventional HPLC columns [4–6]. Twenty-seven fish foods from different companies were analysed using the method and a relationship between the brand's specified astaxanthin concentration in the formulation was interrogated. Prior to analysis, an enhanced and expedited extraction method using methanol with 0.1% acetic acid was employed for direct extraction of AST from fish feed. This method demonstrated strong alignment with industry-standard protocols, offering improved efficiency and performance. Precision was evaluated with respect to retention time, and peak shape showing that the RFS affords improved peak capacity despite affording a separation time half that of the traditional column approach. This simplified extraction and rapid separation approach not only advances AST analysis in fish feeds but also promotes environmental benefits by reducing analysis time and resource consumption.

Keywords: Radial flow splitting, astaxanthin, liquid chromatography, mass spectroscopy.

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DEVELOPMENT OF GREEN AND ROBUST LIQUID CHROMATOGRAPHIC METHOD FOR SIMULTANEOUS DETERMINATION OF AMLODIPINE BESYLATE, PERINDOPRIL TERT-BUTYLAMINE, AND ATORVASTATIN CALCIUM

Amtul Qayoom^{a*}, Saeeda Nadir Ali^a, Raees Anis^a, Shaz Asrar^a, Ghina Mumtaz Alavi^a

^aDepartment of Chemistry, NED University of Engineering and Technology, Karachi-75270, Pakistan.

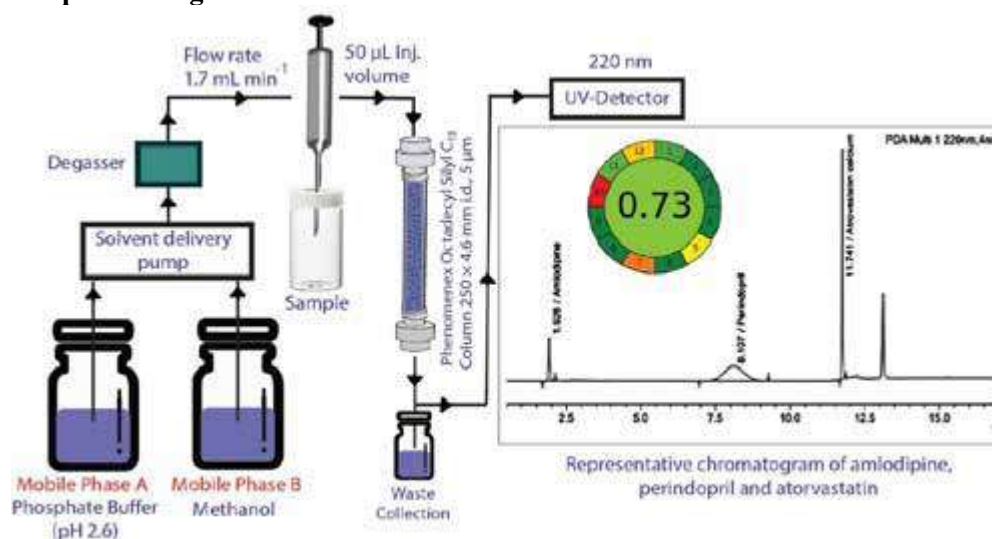
*Corresponding author: amtulq@neduet.edu.pk

Abstract

This study presents a liquid chromatographic technique for the simultaneous determination of amlodipine besylate, perindopril tert-butylamine, and atorvastatin calcium in bulk and pharmacological formulations. HPLC analysis utilized a Phenomenex Octadecyl Silyl column (250 mm x 4.6 x 5 μ m) with a phosphate buffer (pH 2.6): methanol as mobile phase, at a flow rate of 1.7 mL min⁻¹ with gradient elution. Validity of the method was confirmed following ICH guidelines, demonstrating excellent linearity ($R^2 > 0.9975$) over concentration ranges of 10-50, 8-40 and 10-50 μ g mL⁻¹ for amlodipine besylate, perindopril tert-butylamine, and atorvastatin calcium, respectively. RSD values below 2.0%, at all concentration levels suggested satisfactory precision. Percent recovery of all the analytes ranged from 99.59 to 101.43%, which exhibited good accuracy. The robustness of the developed method was also studied, using the Plackett Burman Design. Results suggested that the developed method is reasonably robust for most of the responses however a precautionary statement about flow rate and wavelength of the detector needs to be included in the procedure. The environmental impact of the developed method was assessed using NEMI, AES, and AGREE tools while the method applicability was verified through analysis of analyte in dosage formulations.

Keywords: Amlodipine besylate, Perindopril tert-butylamine, Atorvastatin calcium, HPLC, Plackett Burman Design

Graphic / Image



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ADVANCED DIFFERENTIATION OF BOVINE AND PORCINE IN GELATINE FOR HALAL COMPLIANCE USING LC-MS/MS: A COMPLEMENTARY APPROACH TO DNA-BASED METHODS

Fathiah Ahmad Zubaidi, Farah Idwani Abd Rahman, Hasni Harun

Department of Chemistry Malaysia, Petaling Jaya, Selangor, Malaysia

Corresponding author: fathiah@kimia.gov.my

Abstract

Ensuring Halal compliance in food products requires accurate identification of gelatine sources, particularly when addressing religious and regulatory constraints associated with porcine materials. DNA-based methods, while widely utilized, are often limited in applications involving highly processed foods due to DNA degradation. This study presents a novel Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) method for the simultaneous detection of bovine and porcine biomarkers in gelatine, offering a complementary solution to DNA-based techniques.

The developed peptide-based LC-MS/MS approach demonstrates exceptional sensitivity and specificity, overcoming the challenges posed by complex food matrices. The qualitative approach enables the reliable detection of porcine materials, adhering to stringent Halal requirements that prohibit even trace amounts. Validation results showed outstanding linearity ($R^2 > 0.990$), precision ($RSD < 20\%$), and recovery (80–120%), with limits of detection as low as 0.37–0.95 ng/ml. Real sample applications further validated its effectiveness across diverse food samples, establishing it as a reliable tool for food authenticity testing and Halal compliance verification.

This presentation underscores the innovative use of LC-MS/MS as a complementary method to DNA-based analysis, offering a deeper understanding of its analytical strength and future potential in addressing food authentication challenges.

Keywords: Halal compliance, LC-MS/MS, bovine, porcine, food authentication (gelatine).

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AUTHENTICATION ANALYSIS OF AGARWOOD OIL BY GC-MS USING CHEMOMETRIC APPROACH

Wan Farah Nasuha Wan Iskandar^{a*}, Mohamad Izharudin Che Amat^a, Siti Sarah Abdul Aziz^a and Suraya Hani Ramli^b

^a*Research & Instrumentation Section, Department of Chemistry Malaysia, 46661 Petaling Jaya, Selangor, Malaysia*

^b*Laboratory Services Division, Department of Agriculture, Blok C, Jalan Gallagher, 50480 Kuala Lumpur*

**Corresponding author: farahnasuha@kimia.gov.my*

Abstract

Agarwood oil, an aromatic essential oil derived from the resinous heartwood of *Aquilaria* trees, is highly valued in the perfume and medicinal industries. However, the increasing demand and high market value have led to the emergence of counterfeit and adulterated agarwood oils, often mixed with synthetic or low-quality substitutes. This study employs Gas Chromatography-Mass Spectrometry (GC-MS) combined with chemometric techniques to determine the authentication of agarwood oils. The chemical compositions of 10 oil samples, including 5 agarwood oils and 5 non-agarwood oils, were analyzed using GC-MS. Ten major chemical compounds were selected as critical markers for authentication, with sesquiterpenes and sesquiterpenoids contributing significantly to the distinctive woody aroma of agarwood. Variations in chemical profiles were examined to differentiate authentic and non-authentic samples. These findings demonstrate that integrating GC-MS with chemometric analysis provides a reliable approach for agarwood oil authentication, enhancing quality control and combating adulteration in the industry.

Keywords: agarwood oil; GCMS analysis; boxplot; minitab

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A SELF-CLEANING STRATEGY FOR ELECTROCHEMICAL OXIDATION OF α -PINENE WITH MINIMAL ELECTRODE FOULING

Danny K.Y. Wong*, Zeheng Lin, Joshua Abbott, Peter Karuso, Soo Jean Park

Department of Applied Biosciences, Macquarie University, Sydney NSW 2109, Australia.

*Corresponding author: Danny.Wong@mq.edu.au

Abstract

This work focusses on the electrochemical oxidation of α -pinene, a key semiochemical found in plants, insects, and other organisms that plays a vital role in ecological interactions within natural environments¹⁻³. This study may then aid in developing a sensitive and selective method for field monitoring of α -pinene. In our work, by coupling electrochemistry with spectroscopy, we have identified 4,6,6-trimethyl-bicyclo [3.1.1] hept-3-en-2-one and N-(4,6,6-trimethyl-bicyclo [3.1.1] hept-3-en-2-yl) acetamide as the primary oxidation products of α -pinene at a glassy carbon electrode in the presence of the ionic liquid 1-ethyl-3-methylimidazolium ethyl sulfate ([EMIM][ESO₄]) in acetonitrile as a supporting electrolyte. However, accumulation of these oxidation products at the electrode surface was found to hinder the oxidation of α -pinene, leading to severe electrode fouling that significantly compromised detection sensitivity and accuracy. Meanwhile, cyclic voltammetry of an electrolyte consisting of a similar imidazole-based ionic liquid at an electrode is known to involve the oxygen–superoxide redox reactions⁴. In this work, we have exploited these redox reactions in a self-cleaning protocol to generate a reproducible electrode surface for the oxidation of α -pinene. This strategy effectively prevents detection signal degradation over repeated electrochemical scans, making it feasible to detect α -pinene through multiple oxidation scans. This fundamental work is expected to advance the current understanding of α -pinene electrochemistry, while offering guidelines for the design of robust electrochemical sensors for detecting volatile organic compounds that are essential for environmental and biosecurity monitoring.

Keywords: electrochemical α -pinene oxidation, electrode fouling, self-cleaning strategy

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AI-ASSISTED SMART ANALYTICAL APPROACHES FOR THE EARLY DIAGNOSIS AND PROGNOSIS OF HEART ATTACK

Sook Mei Khor^{a*}, Joyce Siew Yong Low^a, T. Malathi Thevarajah^b, Siow Wee Chang^c

^aDepartment of Chemistry, Faculty of Science, Universiti Malaya, 50603, Kuala Lumpur, Malaysia.

^bDepartment of Pathology, Faculty of Medicine, Universiti Malaya, 50603, Kuala Lumpur, Malaysia.

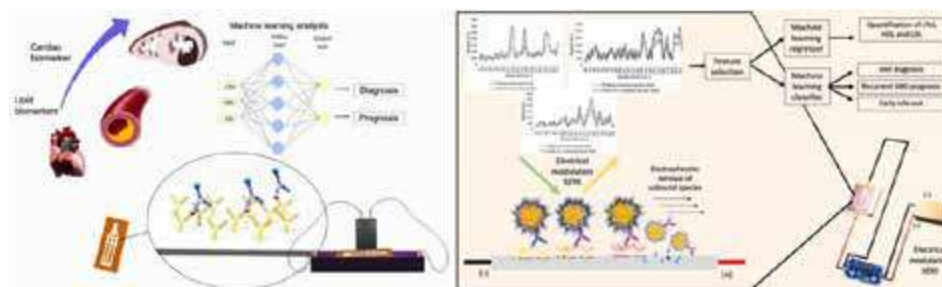
^cInstitute of Biological Sciences, Faculty of Science, Universiti Malaya, Kuala Lumpur, Malaysia.

*Corresponding author: naomikhor@um.edu.my

Abstract

AI-assisted paper-based microfluidic biosensors with optical colorimetric and surface-enhanced Raman scattering (SERS) detection can aid in the rapid and accurate early diagnosis and prognosis of acute myocardial infarction (AMI). The biosensors developed can provide on-site measurements of multiplexed biomarkers, including cardiac troponin (cTnI), high-density lipoprotein (HDL), and low-density lipoprotein (LDL), in the context of AMI. Past studies confronted obstacles or limitations, such as measuring only a single biomarker or total cholesterol levels, which cannot distinguish between LDL and HDL. Colorimetric detection is inexpensive, practical, and does not require complex central laboratory equipment. SERS is a sensitive method used to detect very small amounts of biomarkers, like cardiac troponin, in serum samples. It is particularly useful for early diagnosis. The electrophoretic technique was integrated with the paper-based sensing system to eliminate multiple washing processes that could have slowed the detection time. Non-specifically adsorbed biomolecules, colorimetric tags, or SERS tags can be eliminated from the sample matrix along with the electric field. A machine learning model was added to the data analysis to improve the prediction of AMI attack recurrences. Combining machine learning algorithms such as CatBoost and a new machine learning framework further improves the early diagnosis and prognosis of AMI compared to conventional statistical methods. Any cumbersome apparatus or time-consuming imaging procedures requiring additional resources and turnaround time can be omitted. In short, AI-assisted handheld biosensors enable clinicians to make quicker decisions based on the essential biomarker measurements presented, thereby improving the prognosis of patients through the implementation of prompt medical interventions.

Keywords: Multiplexed analysis; Paper-based biosensor; Early diagnosis and prognosis; Machine learning



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NOVEL INSIGHTS INTO THE PROPERTIES OF STAR ANISE POLYSACCHARIDES AND THEIR POTENTIAL FOR METABOLIC DISORDER MANAGEMENT

Abu Hurairah Darwisy Alias, Muhammad Hakimin Shafie*

*Analytical Biochemistry Research Centre (ABrC), Universiti Sains Malaysia, University Innovation Incubator (I²U)
Building, SAINS@USM Campus, Lebuhr Bukit Jambul, 11900 Bayan Lepas, Penang, Malaysia.*

**Corresponding author: hakiminshafie@usm.my*

Abstract

Metabolic disorders, including obesity, hypertension, and diabetes mellitus, pose significant global health challenges. Natural bioactive compounds, such as polysaccharides have gained attention for their therapeutic potential. Star anise (*Illicium verum* Hook. f.) has been widely recognized for its culinary uses and has been applied for medicinal purposes, especially in Southeast Asian region¹. Star anise extracts have been shown to possess various bioactivities such as antimicrobial, anti-inflammatory, and anticancer properties². However, limited scientific studies have investigated the extraction, characterization, and bioactivities of star anise polysaccharides (SAP), particularly their anti-obesity, antihypertensive, antidiabetic, and antioxidant properties. This study optimized SAP extraction using propane alcohol-based deep eutectic solvents (DES) and microwave-assisted extraction (MAE). The extraction was optimized using response surface methodology (RSM) via Box-Behnken design (BBD), with five extraction variables while maximum yield as the response. The optimized conditions resulted in an extraction yield of 5.14%. The physicochemical, structural, functional, and rheological properties of SAP were analyzed, while bioactivities, including enzyme inhibition (i.e., pancreatic lipase, angiotensin-converting enzyme, and α -glucosidase) and antioxidant properties (i.e., free radical scavenging activity and reducing capacity), were evaluated. SAP exhibited total carbohydrate content and protein content of 19.48% and 0.12%, respectively, indicating a high-purity polysaccharide³. SAP was characterized as a pectin-like polysaccharide with acidic properties (pH 3.04) and amorphous structure⁴. SAP also showed high viscosity (44.86 mPa s), oil-holding capacity (14.39%), esterification degree (72.53%), and branching degree (4.04)⁴. SAP demonstrated potent inhibition of pancreatic lipase (86.67%), angiotensin-converting enzyme (73.37%), and α -glucosidase (82.33%), along with antioxidant properties, as shown by ABTS (34.94%) and FRAP (0.56 mM FeSO₄) assays⁴. These findings suggest that SAP possesses strong bioactivities, largely attributed to their physicochemical properties and structural characteristics, making it a promising natural therapeutic agent for managing metabolic disorders. This study also highlights the potential of sustainable extraction methods for developing functional polysaccharide-based treatments.

Keywords: Anti-obesity; antihypertensive; antidiabetic; polysaccharide; star anise.

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AMYLOID- β PEPTIDES INTERACTION WITH CURCUMIN: AFM AND ELECTROCHEMICAL CHARACTERISATION

A.M. Oliveira-Brett*, A.-M. Chiorcea-Paquim and W.B.S. Machini

Department of Chemistry, University of Coimbra, CEMMPRE-ARISE,

3004-535 Coimbra, Portugal

**Corresponding author: brett@ci.uc.pt*

Abstract

Alzheimer's disease (AD) disrupts the brain's ability to function by impairing the communication between neurons, which normally exchange information via electrical impulses and neurotransmitters. This disruption is primarily caused by the build-up of amyloid beta ($A\beta$) plaques, extracellular deposits of $A\beta$ peptides, and neurofibrillary tangles, helical filaments composed of abnormally formed tau proteins. Structurally, the $A\beta$ peptides contain only three electroactive amino acid residues, tyrosine Y^{10} , three histidines H^6 , H^{13} and H^{14} , and methionine M^{35} . Atomic force microscopy (AFM) and differential pulse voltammetry (DPV) have been recognised as fruitful approaches to study the $A\beta$ peptides structure and aggregation mechanisms [1-4]. characterization, and kinetic study of the aggregation of Alzheimer's disease (AD).

The naturally occurring polyphenol curcumin [5] found in turmeric has strong affinity for binding to $A\beta$ peptides, a key feature of AD pathology. Its structure allows curcumin to interact with the hydrophobic regions of $A\beta$ peptides, which are crucial for β -sheet formation, inhibiting $A\beta$ aggregation and fibril formation, destabilizing existing plaques, and reducing neurotoxicity. The time-dependent structural modifications and electrochemical behaviour of human $A\beta_{1-40}$ and $A\beta_{1-42}$ peptides following their interaction with curcumin, using AFM and DPV, was investigated. The results showed that curcumin disrupts and slows the fibrillization process by binding to specific aromatic residues of the $A\beta$ peptides, via curcumin methoxy and hydroxy groups, hindering the conformational changes required for fibril nucleation and elongation. Curcumin targeted binding not only influences the $A\beta$ peptide dynamics, reducing the extent of fibrilization, but also promotes more open configurations that enhance the electron transfer to the electrode surface, consistent with curcumin inducing the formation of soluble toxic species. This dual ability of curcumin to slow fibril formation and induce the formation of unconventional $A\beta$ monomeric, oligomeric, prefibrillar, and flexible fibrillar species, may reduce the toxicity associated with soluble oligomers and fibrillar $A\beta$ aggregates, highlighting curcumin's potential as a therapeutic agent for AD.

Keywords: Amyloid- β peptide, curcumin aggregation, adsorption, oxidation, AFM, voltammetry.

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INNOVATIONS IN ELECTROCHEMICAL SCIENCES THROUGH 3D PRINTING: FROM TAILORED ELECTRODES TO MULTI-FUNCTIONAL PLATFORMS

Simona Baluchová^{a,*}, Martin Šefčík^a, Jan Fischer^a, Josephus G. Buijnsters^b

^a *Department of Analytical Chemistry, Faculty of Science, Charles University, Albertov 6, 128 00 Prague, Czech Republic*

^b *Department of Precision and Microsystems Engineering, Delft University of Technology, Mekelweg 2, 2628 CD Delft, The Netherlands*

*Corresponding author: simona.baluchova@natur.cuni.cz

Abstract

Additive manufacturing, particularly 3D printing, is advancing electrochemical sciences by enabling the fabrication of both novel electrode materials and optimized electrochemical platforms. One promising avenue is the development of customized conductive filaments for fused deposition modeling (FDM)-based 3D printing¹. These filaments, composed of conductive particles embedded in thermoplastic polymers, allow for the fabrication of electrodes with tuneable properties. As a key innovation, we have successfully developed flexible 3D-printed electrodes composed of thermoplastic polyurethane (TPU), carbon nanotubes, and boron-doped diamond (BDD) microparticles².

Beyond electrode fabrication, 3D printing enables the rapid prototyping of electrochemical cells, facilitating the design of multi-functional platforms. As a proof-of-concept, we developed a dual-function electrochemical platform for both sensing and electrochemical degradation. This system targets venlafaxine (VF) and desvenlafaxine (DVF), two widely used antidepressants that are frequently detected in water³. Monitoring these compounds is crucial not only for environmental safety but also in clinical settings to optimize therapeutic dosages and prevent adverse effects. The platform incorporates a free-standing BDD electrode⁴, where both the nucleation and growth sides are accessible – former for sensing, focus of this contribution, and latter for degradation. Optimized detection conditions were achieved for VF and DVF, yielding sub-micromolar detection limits. Both pharmaceuticals exhibited excellent intra- and inter-day repeatability, with signals remaining stable even in the presence of potential interferents. Electroanalytical performance was further validated in synthetic human serum, synthetic urine, and river water, demonstrating the platform's robustness and applicability for both environmental and clinical monitoring.

Looking ahead, this platform can be fully 3D-printed, replacing the BDD electrode with customized FDM-printed conductive electrodes, integrating material innovation with functional electrochemical applications. These advancements highlight the potential of 3D printing in electrochemistry, paving the way for cost-effective, scalable, and application-specific electrochemical technologies.

Keywords: 3D-printing; dual-function platform; electrochemistry; sensing; water pollutants.

Acknowledgement: This research was financially supported by the Charles University Primus program (grant no. PRIMUS/25/SCI/020).

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RETROSPECTIVE ANALYSIS OF VOLATILE ORGANIC COMPOUNDS (VOCs) IN DRINKING WATER

Kar-Weng Chan*

Department of Chemistry Malaysia

**Corresponding author: chankw@kimia.gov.my*

Abstract

Monitoring volatile organic compounds (VOCs) in drinking water is crucial for ensuring its safety. While over 60 VOCs can be found in water, Malaysia's National Drinking Water Guidelines regulate 25, specifying maximum limits at the parts-per-million (ppm) level.¹ Routine monitoring by local enforcement agencies (e.g., the Ministry of Health Malaysia) focuses on trihalomethanes (THMs), encompassing chloroform, bromodichloromethane, dibromochloromethane, and bromoform. The Department of Chemistry Malaysia is entrusted to quantify these compounds using purge-and-trap gas chromatography mass spectrometry (P&T GC-MS). A retrospective study of 1,807 random water samples analyzed from June to December 2024 showed that THM levels were below the permitted limits in all but one instance, which exhibited elevated chloroform. As the laboratory analyzes 25 VOCs in its standard testing protocols, the retrospective data also revealed the presence of methylene chloride, a VOC not routinely monitored, in 9.1% of samples exceeding the 0.02 ppm limit, with the highest concentration of 1.007 ppm. This is concerning due to the known carcinogenic properties of methylene chloride,² even at low concentrations. The potential sources of this contamination warrant investigation. Therefore, we recommend that relevant enforcement agencies investigate this issue and consider including methylene chloride in routine drinking water monitoring if its presence persists at these levels.

Keywords: volatile organic compounds, drinking water, methylene chloride

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IN-SITU MECHANISM CHARACTERIZATION OF ELECTROCHEMICAL REACTIONS VIA DEVELOPMENT OF FLOATING ELECTROSPRAY MASS SPECTROMETRY

Zhenwei Wei^{a,*}, Chengbiao Zhu^a, Xiangyu Wang^{a,b}, Chen Zeng^a

^a College of Chemistry and Molecular Science, Wuhan University

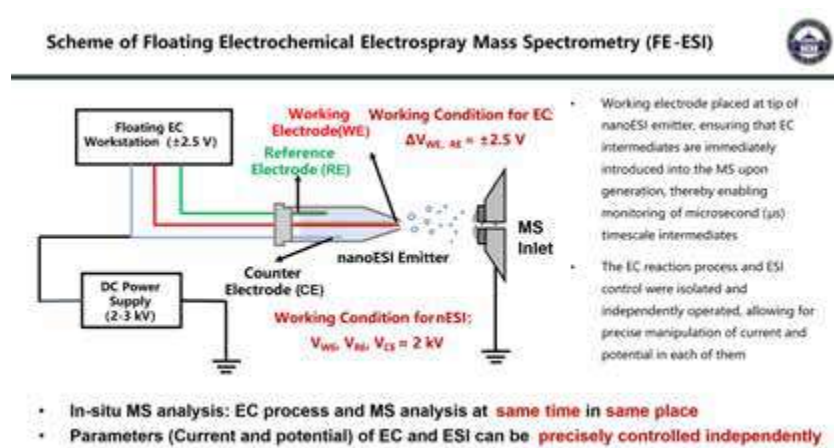
^b School of Public Health, Wuhan University

* Corresponding author: weizw2021@whu.edu.cn

Abstract

The analysis and characterization of reactive intermediates in electrochemical (EC) processes are of great significance for understanding reaction mechanisms and pathways, which is crucial to the rational control of electrochemical synthesis and catalytic processes. Mass spectrometry (MS) is well-suited for qualitative and quantitative analysis of multi-components in complex media; however, conventional MS methods usually need at least second scale time to introduce samples from EC cells to MS, which are unable to perform in situ analysis of active EC intermediates. To solve this problem, we developed a floating electrochemical electrospray ionization mass spectrometry (FE-ESI-MS) system, which can temporally and spatially synchronize the EC process and MS ionization together to enhance in-situ capability of EC-MS analysis [1]. The working electrode was designed to be placed at tip of ESI emitter, which ensured that once the species generated on the working electrode, they can be immediately sent to MS for analysis without any delay. We also solved the interference between EC process and ESI to allow precise control of EC current and potential. This integrated system allowed the analysis and structural identification of intermediates on microseconds timescale. This system has been successfully applied to the rapid screening and mechanistic investigation of electrochemical reactions, such as nitro-reductive coupling and indole radical coupling, leading to the discovery of numerous new intermediates and reaction pathways.

Keywords: electrochemical synthesis and catalysis, in-situ analysis, floating electrospray mass spectrometry, intermediates, reaction monitoring



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EXPANDING THE ELEMENTAL AND ISOTOPIC TOOLBOX IN SUPPORT OF THE SUSTAINABLE DEVELOPMENT GOALS

Johanna IRRGEHER^{a,*},

^aMontanuniversität Leoben, Franz-Josef-Straße 18, 8700 Leoben, Austria

**Corresponding author: johanna.irrgeher@unileoben.ac.at*

Abstract

Atomic spectroscopy has revolutionized the discovery of elements and their isotopes, playing a foundational role in scientific progress with recent milestones like the Avogadro Project and the redefinition of the mole and kilogram.

In addressing the global challenges set forth by the Sustainable Development Goals (SDGs), Analytical Chemistry, particularly inorganic mass spectrometry, assumes a paramount role in providing accurate and reliable data for informed decision-making.

An essential pillar of the scientific community is the Periodic Table of Elements, inseparable from the long-standing Commission on the Atomic Weights and Isotopic Abundances (www.ciaaw.org) within IUPAC. The atomic weights of elements form the bedrock for numerous scientific measurements. Traditionally, determining atomic weights relied on physical methods, with mass spectrometry at the forefront.

During this talk, the potential of modern elemental and isotopic analysis based on (MC)-ICP-(CRC)-MS in environmental-, geo-, life- and materials sciences under consideration of selected sustainable development goals (SDGs 2, 3, 6, 7, 9, 11, 12, 13, 14, 15, 17) will be addressed, as there are many ways chemists are working to support global sustainable development. Recent instrumental developments in ICP-MS will be discussed for elemental as well as isotopic analysis especially emphasizing novel collision and reaction cell technology. Selected projects dedicated to the EU Green Deal and Zero-Waste initiatives will be presented with a focus on inorganic pollutants and substances, such as technology-critical elements. Diverse applications, ranging from harnessing natural isotopic variation to utilizing enriched isotopes, will be discussed, underscoring the crucial role of data processing through isotope pattern deconvolution.

Beyond pure scientific aspects, the talk will delve into the importance of thinking outside the box, exploring alternative perspectives and innovative approaches.

Keywords: mass spectrometry, sustainable development goals, MC-ICP-MS, isotope ratio analysis

RAPID AND ECONOMICAL CHEMOSELECTIVE METABOLOMICS USING BORONATE ESTER FORMATION ON A MONOLITHIC SUBSTRATE

Xiangyu Wang^{a,b}, Peirong Bai^a, Ziying Li^a, Quanfei Zhu^a, Zhenwei Wei^{a,*}, Yuqi Feng^{a,*}

^a College of Chemistry and Molecular Science, Wuhan University

^b School of Public Health, Wuhan University

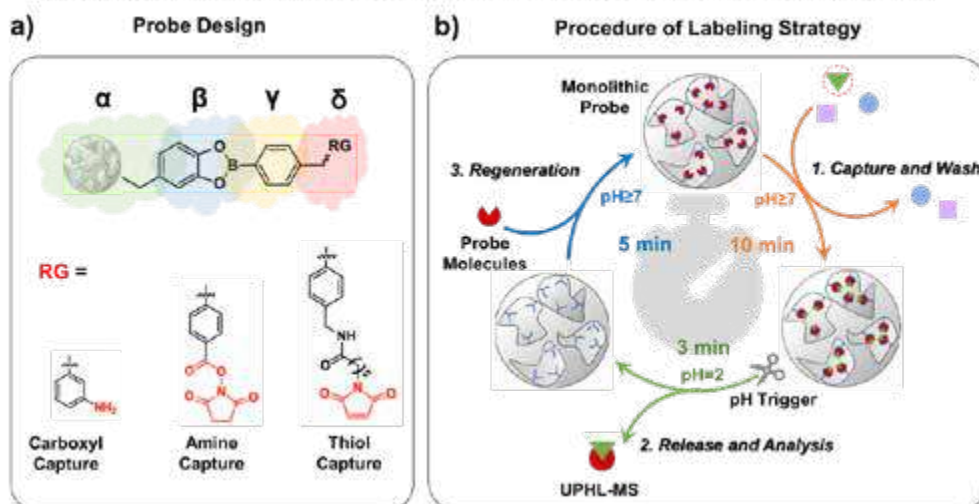
*Corresponding author: weizw2021@whu.edu.cn; yqfeng@whu.edu.cn

Abstract

Although chemoselective labeling strategies show great potential in in-depth description of metabolomics¹⁻³, the associated time and expense limit applications in high-throughput and routine analysis. We report a fast and effective chemoselective labeling strategy based on multifunctionalized monolithic probes⁴. A rapid pH-responsive boronate ester reaction was employed to immobilize and release probe molecules from substrate in 5 min. The mesoporous surface and hierarchically porous channels of the substrate allowed for accelerated labeling reactions. Moreover, the discernible boron beacons allowed for recognition of labeled metabolites with no need for expensive isotopic encoding. This new strategy has been successfully used for submetabolome analysis of yeast cells, serum, and faeces samples, with improved sensitivity for short chain fatty acids up to 1600 times compared with non-labeled liquid chromatography-mass spectrometry (LC-MS) methods.

Keywords: accelerated reactions, chemoselective probes, fast labeling, metabolome analysis

Monolithic Probe and Accelerated Chemoselective Labeling Strategy



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REVOLUTIONIZING BIOMARKER DETECTION: A NOVEL DET-BASED BIOSENSOR WITH AN ANTIBODY-APTAMER HYBRID SANDWICH FOR COMPLEX BIOLOGICAL SAMPLES

Gyeongho Kim^a, Ann Maria K Binu^a, Haesik Yang^{a*},

^aDepartment of Chemistry and Chemistry Institute for Functional Materials,
Pusan National University, Busan, 46241, Republic of Korea.

*Corresponding author: hyang@pusan.ac.kr

Abstract

Direct electron transfer (DET) in electrochemical biosensors enables sensitive, label-free detection. However, its application in sandwich-type biosensors with large antibody-antibody complexes is challenging due to steric hindrance and inefficient electron transfer. Furthermore, the limited availability of high-affinity aptamer-aptamer pairs suitable for complex biological environments further restricts the advancement of DET-based biosensors for clinical use¹. In this study, we developed an electrochemical biosensor that operates via DET using an antibody-aptamer hybrid configuration for sensitive thrombin detection in human serum. An antibody capture probe ensures strong and specific binding to thrombin in human serum, while an aptamer detection probe enables efficient target detection. The aptamer probe is conjugated with a long flexible spacer DNA and a poly-linker peptide containing multiple amine-reactive phenazine ethosulfate (arPES) redox labels, facilitating proximity to the electrode and enhancing electron transfer. Signal amplification is achieved through rapid, repeated DET, leveraging arPES-catalyzed NADH oxidation. The optimized spacer and poly-linker design minimize nonspecific adsorption of the aptamer probe interlinked with multiple arPES and reduce binding interference. Various methods for immobilizing thiol-terminated antibodies on Au electrodes were systematically compared and optimized. The resulting biosensor, based on an antibody-aptamer hybrid sandwich, demonstrated exceptional sensitivity and selectivity in thrombin detection, overcoming the limitations of aptamer-aptamer sandwiches that are hindered by the low affinity of thrombin aptamers in human serum. Remarkably, the biosensor achieved a detection limit of approximately 1.5 pM in buffer and 2.7 nM in human serum, showcasing its potential for precise biomarker detection in complex biological samples.

Keywords: Antibody-aptamer hybrid; Direct electron transfer; Electrochemical biosensor; Multiple redox labels; Thrombin.



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APPLICATION OF CARBON NANOMATERIALS IN ULTRA-TRACE ANALYSIS USING TOTAL-REFLECTION X-RAY FLUORESCENCE SPECTROMETRY

Rafal Sitko^{a,*}, Marcin Musielak^a, Karina Kocot^a, Maciej Serda^a, Beata Zawisza^a

^aInstitute of Chemistry, University of Silesia in Katowice, Szkolna 9, 40-006 Katowice, Poland

*Corresponding author: rafal.sitko@us.edu.pl

Abstract

Total-reflection X-ray fluorescence spectrometry (TXRF) is a powerful micro-analytical technique capable of achieving detection limits in the ng mL⁻¹ range for very small volumes of liquid samples or suspensions (5–10 µL). This method enables multi-elemental ultra-trace analysis using a low-power TXRF instrument without the need for any media, including gases or cooling systems. Consequently, this technique aligns well with the principles of green analytical chemistry. Due to its low operating costs, TXRF is becoming competitive with commonly used spectroscopy techniques such as F-AAS, ET-AAS, ICP-OES, and ICP-MS. However, detection limits of ng mL⁻¹ may often be insufficient for certain applications. Additionally, analyzing samples with complex matrices can be challenging due to increased spectral background, absorption effects, and consequently higher detection limits.

The lecture aims to demonstrate that incorporating carbon nanomaterials, such as graphene, graphene oxide, and carbon nanotubes, in dispersive micro-solid phase extraction (DMSPE) can reduce the TXRF detection limit to the pg mL⁻¹ level. These nanomaterials are noted for their unique properties, including a large surface area, chemical stability, and remarkable adsorption capacity for metal ions [1–3]. However, the adsorption of metal ions on unmodified carbon nanomaterials lacks selectivity, making it difficult to analyze complex sample matrices. The presentation will illustrate that proper surface modification of graphene oxide and carbon nanotubes enhances analyte adsorption and selectivity toward specific metal ions. By using TXRF preceded by DMSPE with carbon nanomaterials, it is possible to achieve detection limits at the pg mL⁻¹ level in a straightforward, rapid, cost-effective, and environmentally friendly manner. The high selectivity of the developed nanomaterials enables the determination and speciation of ultra-trace metal ions in complex matrices, including high-salinity water, plant and biological samples after mineralization, as well as beverages such as juices, wines, and beers without the need for mineralization.

Keywords: TXRF, ultra-trace analysis, nanomaterials, graphene oxide, carbon nanotubes

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INVESTIGATION OF ANTIMICROBIAL EFFECT OF UVC AGAINST *Staphylococcus* spp.

Mohd Yaman Idris^{a,b,*}, Muhammad Afiz Aziz^b,

^a*Jabatan Kimia Malaysia, Jalan Sultan 46661 Petaling Jaya, Selangor Darul Ehsan, Malaysia*

^b*Institute of Biological Sciences, Faculty of Science, Universiti Malaya, 50603 Kuala Lumpur, Malaysia*

*Corresponding author: yaman@kimia.gov.my

Abstract

Staphylococcus spp. are pathogenic bacteria that can cause serious infections and cause a threat to public health. While many studies have shown how to treat and reduce their virulent activities, alternative disinfection approaches should be explored. Hence, our research aims to investigate the efficacy of ultraviolet C (UVC) radiation in inactivating and inhibiting the *Staphylococcus* spp. in vitro. The antimicrobial assay was performed by directly exposing culture plates containing *Staphylococcus epidermidis* (ATCC 35984), *Staphylococcus aureus* (ATCC 25923), and methicillin-resistant *Staphylococcus aureus* (MRSA) (ATCC 43300) to UVC exposure at varying distances (7.5 cm and 19 cm) and durations (30, 60, and 90 seconds).

The drop plate technique was designated in this research, where bacterial suspensions were exposed to UVC radiation on agar plates followed by quantification of colony-forming units (CFUs) after exposure. These results revealed UVC significantly reduced bacterial populations at longer durations and closer distances to the UVC source. Specifically, the finding demonstrates a complete elimination of *S. epidermidis* and MRSA by 100% under UVC exposure of 60 seconds at a distance of 7.5cm. Furthermore, hemolytic and biofilm activities were assessed following UVC exposure and compared to non-exposed controls. It was observed that UVC radiation can suppress bacterial growth at shorter exposure distances.

Overall, our research findings indicate that UVC exposure can be an effective non-chemical disinfection method for healthcare, laboratory, and industrial applications. This study also offers valuable insights into optimizing UVC treatment parameters to enhance environmental and water disinfection strategies.

Keywords: Ultraviolet-C (UVC); disinfection; antimicrobial; biofilm; hemolytic.

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VALIDATION OF DIFFERENTIAL EXTRACTION METHOD FOR SPERM-CONTAINING SAMPLES VIA QIAGEN, QIASYMPHONY SP PLATFORM

Zulhilmi Husni^{a,*}, Nur Fadzlina Yahaya^a, Normazlina Zainudin^a, Siti Hajar Hussin^a, Nor Aidora Saedon^a.

^aDepartment of Chemistry Malaysia.

**Corresponding author: zulhilmi@kimia.gov.my*

Abstract

The study presents the validation of a differential DNA extraction method tailored for sperm-containing forensic samples, using the QIAAsymphony DNA Investigator Kit on the QIAAsymphony SP automated platform. The objective was to evaluate the efficiency of the platform in isolating sperm DNA from mixed biological evidence—typically semen mixed with female epithelial cells—encountered in sexual assault cases. Mock samples were created using various semen-to-female blood ratios (1:10, 1:50, 1:100, 1:500, and 1:1000), and processed using proteinase-K with dithiothreitol (DTT) to disrupt the protamine-protected sperm nuclei.

Validation parameters including sensitivity, repeatability, and reproducibility were assessed. Quantitative PCR (qPCR) and capillary electrophoresis confirmed successful removal of female DNA, with high sensitivity in detecting male DNA even at low semen ratios. Sperm fractions at ratios up to 1:100 yielded clear male DNA profiles, while ratios of 1:500 and 1:1000 still allowed detection, albeit with diminished interpretability due to minor male contribution. Repeatability and reproducibility studies demonstrated consistent DNA yields and profiling results ($p < 0.05$), except for minor variability in epithelial fraction quantification.

The automated QIAAsymphony-based method markedly reduced manual handling and overall processing time—from two days to approximately two hours—through integration of robotic sample processing steps. This optimized approach enhances forensic DNA workflow efficiency, particularly for high-throughput casework, offering reliable and reproducible results with minimal analyst-dependent variability.

Keywords: Differential Extraction, QIAAsymphony SP, Sperm DNA Isolation, Forensic DNA Analysis, Sexual Assault Evidence.

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AN ALTERNATIVE WORKFLOW IN IDENTIFICATION OF MITRAGYNE IN KRATOM SAMPLES BY RADIANT ASAP DIRECT MASS DETECTOR

Nor Fatimah Sameon*, Yasmin Syahirah Noor Azman, Nur Farisha Aina Mohd Anazen, Sharani Abu Samah, Dr. Vanitha Kunalan

Forensics Science Analysis Center, Department of Chemistry Malaysia, Petaling Jaya, Selangor.

*Corresponding author: norfatimah@kimia.gov.my

Abstract

Kratom, scientifically known as *Mitragyna speciosa*, is an indigenous plant commonly found in countries such as Malaysia, Indonesia, and Thailand. Over the years, the abuse of this plant has been discussed and studied in many countries, as it can produce opioid and stimulant-like effects on consumers, especially when taken at uncontrolled dosages. In Malaysia, commonly seized kratom is found in leaf and beverage form, and the processing of kratom leaves and kratom products is still considered illegal due to the harm it causes. Literature study showed a variety of routine instruments have been used for qualitative analysis (e.g., Gas Chromatography-Mass Spectrometry (GC-MS)) and quantitative analysis (e.g., High-Performance Liquid Chromatography (HPLC)) for seized kratom samples (leaves and kratom beverage). However, longer and more tedious sample preparation is required before analysis using these routine instruments to obtain high throughput and optimal results. In this study, a new instrument, known as the RADIANT ASAP Direct Mass Detector was used to determine the presence of mitragynine, the active compound responsible for producing opioid and stimulant-like effects. Three different types of kratom samples (fresh leaves, brown beverage, and mixed beverage) were chosen for this study, taken from real caseworks received by the Narcotic Division, Headquarters of the Department of Chemistry Malaysia. The selected samples have been previously analyzed using GC-MS and confirmed to contain mitragynine. The findings showed that the RADIANT ASAP Direct Mass Detector was able to detect the presence of mitragynine in all three types of samples. These findings highlight a new, robust, and less time-consuming method requiring less sample preparation for the identification of mitragynine compared to commonly used methods. Thus, this method offers a promising and reliable analysis for combating the abuse of kratom in the future.

Keywords: Kratom, *Mitragyna speciosa*, mitragynine, RADIANT ASAP Direct Mass Detector

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CHARACTERISATION OF X-CHROMOSOMAL SHORT TANDEM REPEAT OF CHINESE PERANAKAN IN MALACCA, MALAYSIA

Muhamad Sufiyan Azah^{a,b}, Sharifah-Nany Rahayu-Karmilla Syed-Hassan^{b*}

^a*Department of Chemistry Malaysia Terengganu State, Jalan Alif 1, Wakaf Beruas, 20050 Kuala Terengganu, Terengganu, Malaysia.*

^b*Department of Pathology and Medical Laboratory, Faculty of Medicine, Medical Campus, Universiti Sultan Zainal Abidin, Jalan Sultan Mahmud, 20400 Kuala Terengganu, Terengganu, Malaysia.*

**Corresponding author: karmillahassan@unisza.edu.my*

Abstract

X-chromosomal short tandem repeats (X-STRs) have become a part of tools in forensic and populations genetics studies. Utilization of X-STRs profiling kit such as the Investigator Argus X-12 QS kit, as one of the key components in the downstream processing using advanced analytical tools enable accurate STR profiling, has been proven to leverage forensic casework processing and ancestral inference. The study aims to explore the initial characteristics of X-STRs in an admixed population and evaluate the forensic parameters, despite their distinct genetic makeup. A total of 80 individuals of Chinese Peranakan were sampled from Malacca. Genomic DNA was extracted and amplified using the Investigator Argus X-12 QS kit following standardized protocols. Forensic statistical analyses were performed to calculate key parameters in population databases. Comparative analyses were conducted using reference datasets from the established Malaysian Malay, Chinese and Indian population database of X-STRs. Early trends of reported Singapore's Chinese Peranakan ancestral estimation indicate ancestral a fusion of Malay and Chinese Mainland at certain percentage, demonstrating an admixed event that occurred and support the historical claims of inter-marriage between Chinese and Malay. Establishing this X-STR database will not only bolster forensic identification capabilities but also contribute to our understanding of the genetic ancestry in a culturally significant and underrepresented group—an endeavour that aligns with the analytical advances and challenges currently faced in forensic genetics.

Keywords: X-chromosomal short tandem repeats, Chinese Peranakan, population database, forensic genetics

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AI-GUIDED SMART CHROMATOGRAPHY SYSTEM

Fanyang Mo^{a*}, Boxuan Zhao^b,

^a School of Materials Science and Engineering, Peking University, 100871, Beijing, P. R. China.

^a School of Advanced Materials, Peking University Shenzhen Graduate School, Shenzhen, 518055, China

^b School of Materials Science and Engineering, Peking University, 100871, Beijing, P. R. China.

*Corresponding author: fmo@pku.edu.cn

Abstract

Preparative column chromatography and preparative thin layer chromatography (TLC) are vital separation techniques in synthetic chemistry, yet they are hindered by high trial-and-error costs and labor-intensive, time-consuming procedures that reduce research efficiency. To alleviate these challenges, we are developing intelligent separation solutions using artificial intelligence (AI) and automation¹⁻³.

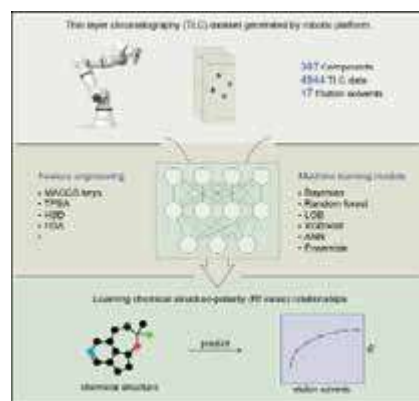
We have created comprehensive experimental platforms that automate the entire separation workflow. Our fully automated chromatography system handles all steps—from sample loading, fraction collection, pooling, and concentration to complete solvent removal. With a sample loading step, multiple samples are processed simultaneously to yield purified compounds. Similarly, our automated preparative TLC platform achieves precise spotting, high-throughput development, automated identification, scraping, and collection of sample spots from silica gel plates, greatly improving efficiency and safety.

The high-quality data generated by these platforms enable us to tackle the complexities of chromatographic separations. Leveraging artificial intelligence, we can accurately predict outcomes for both TLC and column chromatography, significantly reducing the trial-and-error costs of optimizing conditions and advancing the process from automation to true intelligence. With integrated AI models, our column chromatography platform automatically determines optimal conditions based on the compounds, detects anomalies during separation, and promptly adjusts strategies to ensure stable, efficient purification. Concurrently, the automated TLC platform further enhances its intelligence by precisely predicting R_f values, facilitating automatic target identification and efficient collection.

This integrated approach not only streamlines the separation process but also improves reliability and throughput, ultimately advancing synthetic chemistry by allowing researchers to focus on innovation rather than routine operational tasks.

Keywords:

Preparative column chromatography, thin layer chromatography, artificial intelligence, automation,



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COMPREHENSIVE INVESTIGATION OF GRAPHENE OXIDE FOAM AND GRAPHENE OXIDE FUNCTIONALIZED WITH β -CYCLODEXTRINS FOR THE PRECONCENTRATION AND DETERMINATION OF URANYL IONS

Karina Kocot^{a*}, Rafal Sitko^a

^aUniversity of Silesia in Katowice, Katowice, Poland

*Corresponding author: karina.kocot@us.edu.pl

Abstract

The precise and sensitive determination of uranyl ions (UO_2^{2+}) is of paramount importance for environmental monitoring, nuclear industry safety, and public health, largely due to the considerable toxicity and radioactivity associated with uranium compounds¹. As a heavy metal, uranium can pose significant risks to ecosystems and human health when present in contaminated sites, necessitating effective analytical methods for its detection. Despite substantial advancements in spectroscopic techniques over recent decades, the direct detection of low concentrations of uranyl ions in various environmental matrices remains a significant analytical obstacle^{2,3}.

The study focuses on the utilization of graphene oxide foam (GOF) and graphene oxide (GO) modified with β -cyclodextrins (GO- β -CD) for the preconcentration and subsequent determination of uranyl ions by energy-dispersive X-ray fluorescence (EDXRF) and total-reflection X-ray fluorescence (TXRF). The presentation will show the advantages of X-ray spectroscopy measurement in comparison with conventional atomic spectroscopy detection. The evaluated procedures are simple, efficient, and goes in pair with basic principles of green analytical chemistry since it does not require toxic organic solvents and utilizes low energy per sample consumption.

Parameters influencing uranyl ion adsorption were comprehensively assessed. The effectiveness of the GOF and GO- β -CD materials in preconcentrating uranyl ions was evaluated through detailed kinetic studies and adsorption isotherms, which provide insights into the adsorption mechanisms and capacity. Furthermore, the validation of the proposed analytical procedure was rigorously conducted using authentic environmental samples, underscoring its applicability and reliability in real-world scenarios.

Keywords: uranyl ions, graphene oxide foam, graphene oxide- β -cyclodextrin, preconcentration, X-ray fluorescence spectrometry

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DNA EXTRACTION FROM SKELETAL HUMAN REMAINS USING MAGNETIC BEAD-BASED EXTRACTION AND ORGANIC EXTRACTION

Mahzan Md Tab^{a*}, Mohd Nazwantul Idlan Mohammad Rushle^a, Dayang Zarifah Atailah Awang Aemeran^a, Faten Najah Mohd Kassim^a, Nur Fadzlina Yahaya^a, Siti Hajar Hussin^a & Nor Aidora Saedon^a

^aDepartment of Chemistry Malaysia, Petaling Jaya

*Corresponding author: mahzan@kimia.gov.my

Abstract

DNA extraction from skeletal remains is critical for forensic casework, particularly in cases involving degraded biological evidence. This study evaluates and compares organic extraction (phenol-chloroform method) and magnetic bead-based extraction using the EZ1 & EZ2 DNA Investigator Kit via automated EZ2 Connect Fx instrument. A key focus is on reducing turnaround time for forensic DNA cases while ensuring optimal DNA yield and purity. The research examines several bones types, including femur, petrous bone, sternum, teeth, and ribs, with varying incubation periods to assess the efficiency of each method. Results indicate that while organic extraction yields higher DNA quantities, the overall DNA quality remains comparable between methods. However, the organic extraction process is significantly more time-consuming and labour-intensive. In the meantime, the difference between two pre-treatment processes applied has also being studied; 2-hrs and 16-hrs incubation period and tested via EZ2 Connect Fx protocol. The findings showed that the DNA obtained from the 2-hrs incubation period were comparable with the 16-hrs (overnight), indicating that a shorter pre-treatment period is sufficient to produce optimum and reliable results. These results demonstrated that the 2-hrs incubation period via automated EZ2 Connect Fx instrument protocol is highly adoptable to improve turnaround time for Forensic DNA cases especially in the Disaster Victim Identification (DVI). Additionally, the automated EZ2 Connect Fx system enhances DNA recovery, facilitates effective isolate accumulation, and improves the chances of successful human identification. These findings contribute to refining forensic workflows and advancing skeletal DNA analysis.

Keywords: skeletal remains DNA analysis, magnetic bead-based extraction, organic extraction (phenol-chloroform method), automated instrument

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HIGH-THROUGHPUT SINGLE-CELL STRUCTURAL LIPIDOMICS

Xiaoxiao Ma^{*}, Chenxi Cao, Simin Cheng

Department of Precision Instrument, Tsinghua University

**Corresponding author: maxx@tsinghua.edu.cn*

Abstract

Single-cell mass spectrometry (MS) enables sensitive, multiplexed analysis of metabolites and lipids, advancing cell phenotyping and pathway studies. However, lipid structural identification in individual cells remains challenging due to limited sample volumes, especially in high-throughput scenarios, where there is a need to balance the total analysis time per cell with the number of tandem MS (MS/MS) acquisitions. This study aims to develop a high-throughput method for resolving lipid structures in single cells while maintaining rapid analysis rates and structural specificity. A Waters quadrupole-cyclic ion mobility-time-of-flight MS (Q-Cyclic IM-TOF-MS) was employed. Single cells were introduced via a custom three-layered capillary tubing (CyESI). Precursor ions from single cells were separated using cyclic ion mobility, followed by full-scan or co-fragmented spectral acquisition. Specifically, IM-MS and IM-MS/MS spectra were generated using low/high collision energy frames. A nonnegative least square optimization algorithm deconvoluted MS/MS data based on lipid-specific ion mobility elution times, allowing for accurate identification and quantification of lipid species. The workflow achieved a throughput of 29 cells/minute. From single MDA-MB-468 cells, 15 and 36 lipids were identified in positive and negative ion modes, respectively. Resuspending cells in ammonium bicarbonate enhanced *sn*-position resolution for phosphatidylcholines, increasing negative-mode identifications to 45 species. This method establishes a high-throughput platform for single-cell lipidomics, enabling detailed structural identification of lipids. The integration of cyclic IM, wide-window MS/MS, and computational deconvolution addresses critical challenges in single-cell analysis.

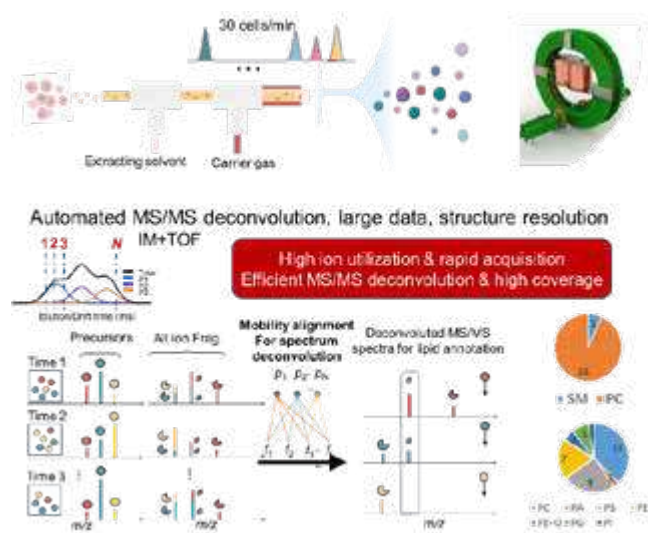


Figure 1. The High-throughput MS analysis system for single-cell structural lipidomics

Keywords: Single-cell lipidomics, High-throughput analysis, Structural identification.

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DUAL-MODE ADSORPTIVE AND ELECTROCHEMICAL SENSING OF BISPHENOL A USING HYBRID CONDUCTING POLYMER-CHITOSAN MAGNETIC NANOPARTICLES

Kavirajaa Pandian Sambasevam^{a,b*}, Adrina Zulkifli^a, Siti Nor Atika Baharin^a,
Zainiharyati Mohd. Zain^b, Wan Jefrey Basirun^c

^aAdvanced Materials for Environmental Remediation (AMER), Faculty of Applied Sciences, Universiti Teknologi MARA, Cawangan Negeri Sembilan, Kampus Kuala Pilah, 72000 Kuala Pilah, Negeri Sembilan, Malaysia

^bElectrochemical Material and Sensor (EMaS) Research Group, Universiti Teknologi MARA, Shah Alam, 40450 Selangor, Malaysia.

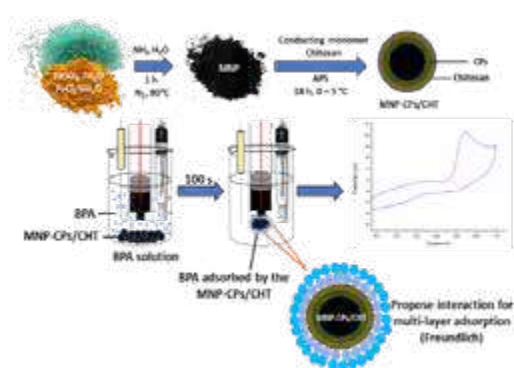
^cDepartment of Chemistry, Faculty of Science, Universiti Malaya, 50603, Kuala Lumpur, Malaysia

*Corresponding author: kavirajaa@uitm.edu.my

Abstract

Bisphenol A (BPA) is an endocrine disruptor commonly found in contaminated water sources, posing risks to human health and wildlife. Effective detection and removal methods are crucial, yet current approaches often lack dual functionalities for both high adsorption capacity and electrochemical sensing. In this study, hybrid conducting polymer/chitosan-based magnetic nanoparticles (MNP-CPs/CHT) were developed for simultaneous BPA adsorption and electrochemical sensing using a magnetic carbon paste electrode (MCPE). MNPs were synthesized via a co-precipitation method, followed by the polymerization of a conducting monomer (typically polyaniline or polypyrrole) and chitosan onto the magnetic core to produce MNP-CPs/CHT. The material was characterized using FTIR, XRD, FESEM-EDX, and VSM. UV-Vis spectroscopy was employed to study the adsorption kinetics, isotherms, and thermodynamics of BPA on MNP-CPs/CHT, revealing temperature-dependent adsorption with a maximum uptake at 318.15 K. The adsorption kinetics followed a pseudo-second-order model, while the adsorption isotherm followed a Freundlich model, indicating heterogeneous adsorption on active sites. The activation energy was determined to be $-132.89 \text{ kJ mol}^{-1}$, which may require further validation as physisorption typically involves lower activation energy. BPA detection on MNP-CPs/CHT-modified MCPE was optimized by investigating different electrolytes, pH levels, and scan rates. Cyclic voltammetry showed that MNP-CPs/CHT exhibited the highest current response, indicating enhanced electron transfer capability and a highly conductive surface for BPA detection. Differential pulse voltammetry (DPV) enabled BPA detection within a linear range of $1\text{--}100 \text{ }\mu\text{M}$, with a detection limit of 0.36 nM . The sensor demonstrated excellent reproducibility, selectivity, stability, and high recovery rates in real water samples, with recovery values within an acceptable range. This study highlights that MNP-CPs/CHT provide a low-cost, efficient solution for BPA detection, offering an integrated approach to addressing environmental and public health challenges associated with BPA contamination in water.

Keywords: Adsorption, BPA, electrochemical sensing, MCPE, MNP-CPs/CHT



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ISOMER-LEVEL STRUCTURAL RESOLVING OF LIPIDS

Suming Chen^{a,*}, Guifang Feng^a, Rongrong Fu^a, Yuhao Han^a

^aThe Institute for Advanced Studies, Wuhan University, Wuhan, Hubei 430072, China

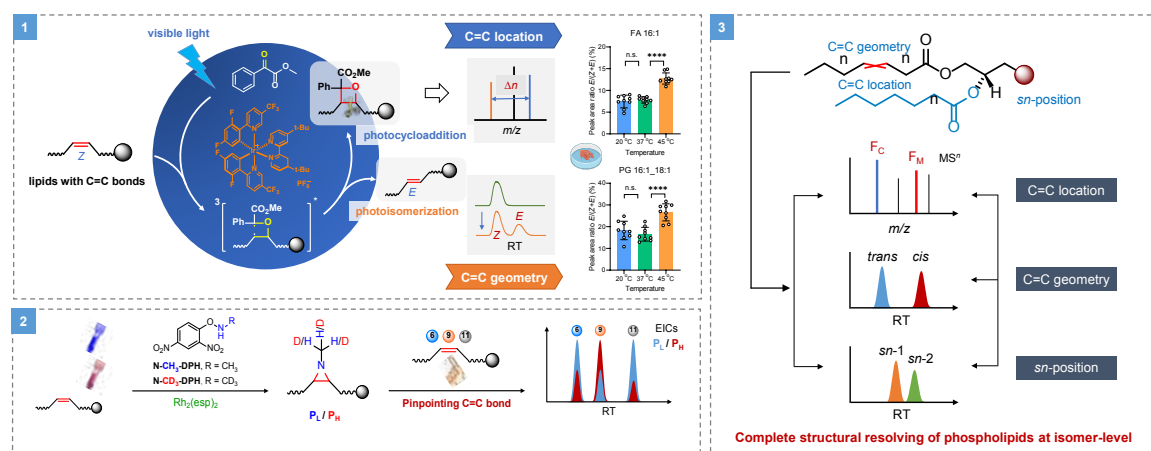
*Corresponding author: sm.chen@whu.edu.cn

Abstract

Lipids are known to contain different forms of isomers, and these structural isomers differ greatly in their biological function. Our group has aimed to develop novel strategies to address the challenges of complete structure resolution of complex lipids at the isomer-level, providing key tools for the biological function study of lipid isomers.¹⁻⁴

1. We developed a bifunctional visible-light-activated photocycloaddition-photoisomerization reaction system, which enables the dual-resolving of the positional and geometric isomerism of C=C bonds in lipids when combines with liquid chromatography-mass spectrometry. Based on this bifunctional reaction system, a workflow of deep structural lipidomics is established, and allows the revealing of unique patterns of *cis-trans*-isomers in bacteria, as well as the tracking of C=C positional isomers changes in mouse brain ischemia.
2. We developed a novel stable-isotope N-Me aziridination strategy that enables simultaneous qualification and quantification of unsaturated lipid isomers. The one-step introduction of the 1-methylaziridine structure not only serves as an activating group for the C=C bond to facilitate positional identification but also as an isotopic inserter to achieve accurate relative quantification.
3. We developed a new strategy for multidimensional lipid structure analysis towards the complete structure resolution of complex lipids, which can realize the simultaneous and precise identification of lipid C=C bond position, C=C bond configuration and *sn*-position.

Keywords: Lipid isomers; Structural lipidomics; Mass spectrometry; *Cis-trans*-isomers; Aziridination



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RAMAN SPECTROSCOPY: A POWERFUL TOOL IN IDENTIFICATION OF DRUGS FOR HIGH WORKLOAD LABORATORY

**Harlisa binti Haidhir Harminder^{a,*}, Siti Zubaidah binti Mohd Yusoff^a, Dr.Saravana Kumar^a,
Dr.Vanitha Kunalan^a**

^aNarcotic Division, Department of Chemistry Malaysia, Jalan Sultan, 46661, Petaling Jaya, Selangor.

**Corresponding author: harlisa@kimia.gov.my*

Abstract

RAMAN Spectroscopy has emerged as a powerful analytical technique for the rapid and non-destructive identification of drugs. The onset of the Handheld RAMAN spectrometer has further boosted its applicability by providing portability, ease of use and real-time analysis capabilities. This present study evaluates the performance of Handheld RAMAN Spectroscopy for illicit drugs detection in narcotics case samples. A total of 50 illicit drugs samples of different types were taken from various case works. These samples were previously tested using Gas Chromatography Mass Spectrometry (GCMS) before being reanalysed with Handheld RAMAN Spectroscopy. The methodology involves spectral data collection from the drug samples, followed by spectral matching against the library database for identification. The results demonstrated the ability of Handheld RAMAN to detect illicit drugs more rapidly than the common analytical technique like mass spectrometry. Its sensitivity offers good detection even in complex mixtures. However, its effectiveness can be reduced when analysing low purity substances. In low purity samples, multiple components contribute to a complex spectrum with overlapping peaks, making it harder to extract the meaningful spectral information. Other challenges such as fluorescence interference are also discussed in this presentation. To conclude, while Handheld RAMAN Spectrometry provides rapid, non-destructive drug analysis and also serves as an effective field-based tool, the performance is significantly challenged by factors such as fluorescence interference, colour, impurities and matrix interferences.

Keywords: Handheld RAMAN Spectrometry, illicit drugs, rapid, low purity, fluorescence

STRUCTURING OF BORON DOPED DIAMOND SURFACES FOR ELECTROANALYSIS

Karolina Schwarzová-Pecková^a, Hana Dejmková^a, Anton Lytvynenko^{a,b}, Lukáš Fojt^c, Miroslav Fojta^c, Jan Hrabovský^b, Andrew Taylor^b

^aDepartment of Analytical Chemistry, Faculty of Science, Charles University, Prague, Czech Republic

^bFZU – Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

^cInstitute of Biophysics, Czech Academy of Sciences, Brno, Czech Republic

*Corresponding author: karolina.schwarzova@natur.cuni.cz

Abstract

Boron-doped diamond represents, after more than 30 years since its discovery, a well-established electrode material for electroanalysis with many applications for the detection of inorganic substances and (bio)molecules [1]. Although polycrystalline BDD films deposited on silicon or metal substrates (*e.g.*, Ti, W, Pt) are most widely used, smooth monocrystalline BDD films or polished films with enhanced electron transfer kinetics have been recently introduced [2]. From the point of view of electroanalysis, structured or porous BDD surfaces may be advantageous due to enhanced sensitivity and lowering detection limits, as well as construction of flow-through sensors for detection in liquid-flow techniques. However, fabrication of such surfaces is challenging due to peculiarities of diamond growth procedure and the inherent properties of the material (hardness, inertness). Most frequently, post-growth structuring or growth employing structured templates has been employed. These approaches may influence the basic characteristics of BDD as sp^2 carbon content or exposed planes of diamond alternate the electrochemical properties of the material. In this contribution, it will be presented on examples of engineered BDD surfaces recently developed by our group, *i.e.*:

1. IR laser-processed polycrystalline and chem-mechanically polished BDD layers [2] leading to micrometer spot-structuring of the surface and controlled introduction of sp^2 carbon, smooth single-crystal {100} BDD layers nanostructured with spherical cavities introduced via microwave plasma chemical vapor deposition in the presence of silica nanosphere templates.
2. To address advantages of these novel BDD varieties, the stability and their physico-chemical properties and prospective applications will be demonstrated via electrochemical detection of dopamine or assessment of adsorptive properties.

Acknowledgements: Financial support from Czech Science Foundation (project GAČR 23-05688S) is gratefully acknowledged.

Keywords: boron doped diamond, electroanalysis, single crystal, surface structuring

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APPLICATION OF MXENES IN SENSORS AND SENSING DEVICES

Arunas Ramanavicius^{a,b*}, Ilya Navitski^b, Sarunas Zukauskas^b, Veronika Zahorodna^c, Viktoriia Korniienko^{d,e}, Simonas Ramanavicius^b, Oleksiy Gogotsi^{c,f}, Maksym Pogorielov^{d,e}, Almira Ramanaviciene^a

^a NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania;

^b Department of Nanotechnology, Centre for Physical Sciences and Technology, Vilnius, Lithuania;

^c Materials Research Center, Kyiv, Ukraine;

^d Biomedical Research Centre, Sumy State University, Sumy, Ukraine;

^e Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia;

^f A.J. Drexel Nanomaterials Institute and Materials Science & Engineering Department, Drexel University, Philadelphia, PA 19104, U.S.A.

*Corresponding author: arunas.ramanavicius@chf.vu.lt

Abstract

Recent progress in the application of new 2D-materials – MXenes – in the design of biosensors, biofuel cells and bioelectronics is evident [1]. Therefore, recent developments in the formation of a relatively new class of 2D metallically conducting MXenes opens a new avenue for the design of conducting composites with metallic conductivity and advanced sensing properties. Advantageous properties of MXenes suitable for biosensing applications [2] will be discussed. Frontiers and new insights in the area of application of MXenes in sensorics, biosensorics and in the design of some wearable electronic devices will be outlined. Some disadvantages and challenges in the application of MXene based structures will be critically discussed. Application of different physicochemical methods in MXene-based sensors will be discussed [3]. Analytical properties of delaminated $\text{Ti}_3\text{C}_2\text{T}_x$ MXene based electrochemical sensor capable of selectively detecting low concentrations of Pb^{2+} in a mixture with other common metal ions, using cyclic voltammetry will be presented. The sensor's performance, such as its sensitivity, limit of detection (LOD), was determined using cyclic voltammetry. The proposed reaction mechanism involves a reversible transition between Pb^{2+} ions and PbO at the MXene layer [4]. The sensors, as prepared, had a linear response range from 0.15 to 2 μM , with a sensitivity of $\sim 20 \mu\text{A}/\mu\text{M}$, and the LOD of $\sim 60 \text{ nM}$.

Keywords: 2D materials; MXenes; TiO_2 nanoparticles; $\text{Ti}_3\text{C}_2\text{T}_x$; Raman spectroscopy.

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ENSURING ACCURACY: VALIDATION OF A MERCURY ANALYZER FOR TOXICOLOGICAL ASSESSMENT IN BLOOD AND URINE

Ridzuan Abd Aziz Mohd Yusop*, Raffiq Izwan Omar, Sharmilah Kuppusami, Ayub Ismail

Toxicology Division, Department of Chemistry Malaysia, Jalan Sultan, 46661, Petaling Jaya, Selangor.

**Corresponding author: ridzuan@kimia.gov.my*

Abstract

Mercury (Hg) is a highly toxic heavy metal that poses significant health risks, necessitating accurate and efficient biomonitoring. The MA-3 Solo, a direct mercury analyser, offers a rapid and cost-effective method without the need for chemical digestion for determining total Hg levels in whole blood and urine. The combination of thermal decomposition, gold amalgamation, and CVAAS technique provides accurate and reliable mercury measurements in whole blood and urine samples. Here, we developed a method and validated in accordance to the ISO-17025:2017 and international standard guidelines ensuring its accuracy, precision, sensitivity, and reproducibility.

Important parameters influencing the analysis process were investigated and optimized. Linearity (0.0-10.0 ng) was with coefficient of determination (r^2) > 0.99. Limit of detection (LOD) and limit of quantification (LOQ) obtained were 0.8 µg/L and 2.8 µg/L for blood and 0.9 µg/L and 3.1 µg/L for urine, respectively. Other parameter assessed were precision which was 2.24% for blood and 2.62% for urine and recovery were 98-113% for blood and 90-106% for urine. The MA-3 Solo demonstrated high sensitivity with low LOD and LOQ values, strong linearity across a working range and excellent repeatability. Recovery rates for blood and urine samples were within acceptable limits, confirming the method's reliability for biological monitoring. These results were found reliable when compared to those obtained using Inductively Coupled Plasma Mass Spectrometer (ICP-MS), which is the gold standard. The results indicate that the MA-3 Solo is a robust and efficient tool for total mercury analysis. Its direct analysis capability, minimal sample preparation, and high throughput provide significant advantages over traditional digestion-based methods.

Keywords: Mercury analysis, blood, urine, validation, toxicology

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AFFINITY-SWITCHABLE BIOTIN BINDING: A NEW SIGNAL TRANSDUCTION APPROACH FOR RAPID MOLECULE ANALYSES

Kui-Thong Tan

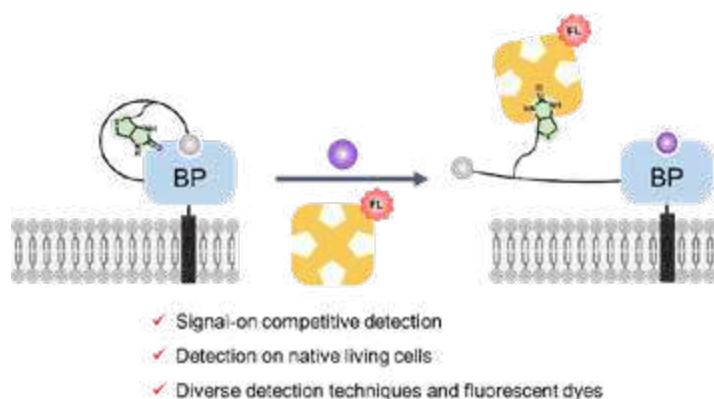
National Tsing Hua University, Taiwan (ROC)

**Corresponding author: kttan@mx.nthu.edu.tw*

Abstract

Currently, genetically encoded protein sensors based on Förster resonance energy transfer (FRET) and circularly permuted fluorescent proteins (cpFPs) are the main strategy used for measuring metabolite concentrations in living cells. However, applications of these protein sensors are restricted to genetically engineered cells. Furthermore, they usually generate only small changes in fluorescence readout with limited selection of fluorophores. In this paper, we introduce a new affinity-switchable biotinylated protein design in which binding of a metabolite target with the protein activates streptavidin-biotin interaction to generate a large 208-fold fluorescence turn-on ratio. In the absence of a small molecule target, the biotinylated protein forms a closed conformation where the biotin is positioned in close proximity to the protein, imposing a large steric hindrance to prevent the effective binding with streptavidin. In the open form, this steric hindrance is removed, thereby exposing the biotin for streptavidin binding. With this sensing concept, various sulfonamides, methotrexate and trimethoprim drugs can be selectively detected on the cell surface of native and genetically engineered cells by using different fluorescent dyes and detection techniques, e.g. fluorescent imaging and flow cytometry. We believe that this affinity-switchable signal transduction strategy can be a versatile tool for rapid, specific and sensitive detection of many other metabolites.

Keywords: Affinity binding, Signal transduction, Molecule analyses, Biotin



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[BMIM]Cl-AGNPS IMMOBILIZED ON EGGSHELL MEMBRANE FOR DETERMINATION OF SULFAMETHOXAZOLE IN ENVIRONMENTAL WATER

Nur Azila Mhd Wahi^{a,*}, Faris Darwish Fadzil^a,
Sharifah Mohamad^a, Arniza Khairani Mohd Jamil^a,

^aDepartment of Chemistry, Faculty of Science,
Universiti Malaya,
50603 Kuala Lumpur, Malaysia.

*Corresponding author: nurazila.mw@gmail.com

Abstract

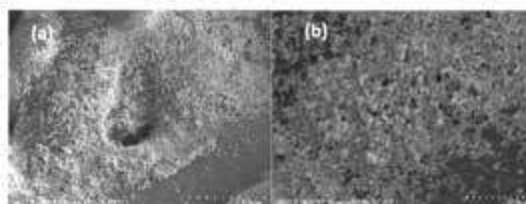
An alternative adsorbent, [BMIM]Cl-AgNPs/ESM, was developed through a simple reduction method and directly immobilized on ESM. It was successfully applied as a solid-phase extraction (SPE) adsorbent for the determination of sulfamethoxazole (SMX) in environmental aqueous samples via HPLC-DAD. Characterization was accomplished by FT-IR and FESEM/EDX. The optimization of [BMIM]Cl-AgNPs/ESM-based SPE method was studied by the one variable at a time (OVAT) approach. Method validation showed good linearity ($R^2 = 0.9995$) in the range of $10 \mu\text{g L}^{-1}$ to $500 \mu\text{g L}^{-1}$, with the detection and quantification limits determined to be $3.07 \mu\text{g L}^{-1}$ and $9.31 \mu\text{g L}^{-1}$ respectively. Additionally, a reusability study showed the developed adsorbent could extract SMX up to three cycles without a significant reduction in its efficiency. Excellent recoveries (90.07 % - 104.08 %) in spiked tap and lake water demonstrate the potential of [BMIM]Cl-AgNPs/ESM for trace level detection of pollutants.

Keywords: ionic liquid silver nanoparticles, eggshell membrane, sulfamethoxazole, solid phase extraction, high-performance liquid chromatography

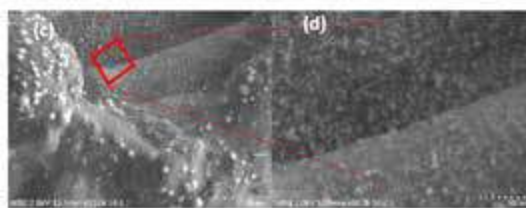
Schematic illustration of [BMIM]Cl-AgNPs/
ESM-based SPE procedure



(a), (b) Newly adsorbent



(c), (d) Reused adsorbent



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UNDERSTANDING MERCURY IN THE PETROLEUM INDUSTRY: A NOVEL ISOTOPE AND SPECIES PREDICTIVE TREND

A.H.Goodman^{a,*}, F.Jaafar Azuddin^a, Zainol.A.Abu Bakar^a, Tg.M.U. B Tg Mat^a, S. Zainal^a.

^a CCUS, Group Technology and Commercialisation,

Petronas Research Sdn Bhd, Jalan Ayer Hitam, 43000 Kajang, Selangor, Malaysia.

*Corresponding author: abigail.goodman@petronas.com.my.

Abstract

Mercury is present in nearly all oil and gas reservoirs, with concentrations ranging from less than 10 parts per billion (ppb) to over 1 part per million (ppm). It exists in four forms: elemental mercury, inorganic salts, organic compounds, and particulate mercury. Elemental mercury is primarily found in hydrocarbon production but can react to form other types. Production data from one of Malaysian fields have revealed unexpected mercury encounters during development, and solutions for better planning and risk management in mercury-affected fields are critical. The objective of the study was to develop a better understanding of mercury's sources, transformation mechanisms, and migration history within the petroleum industry. This was achieved by combining both physical and chemical mercury chemistry whilst leveraging on geological characteristics and specialized analytical methods. A trend was established based on the study by Yin et al and 41 isotopic datapoints from 5 fields which can be linked to Hg forms from the operational speciation. This novel approach to assess Hg origin in field development and migration patterns in the subsurface based on isotopic signatures and estimates of species distribution can be applied in both surface and subsurface application. Further validation to improve the accuracy of the model, will produce future potential to have a predictive tool for Hg distribution.

Keywords: Isotopes, Mercury speciation, Inorganic chemistry, Petroleum Industry.

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ORGANIC MOLECULAR PROBES FOR IMAGING AND THERAPY

Yanli Tang^{a*}, Ling Li^a, Xinyi Zhang^a, Yuxin Ren^a

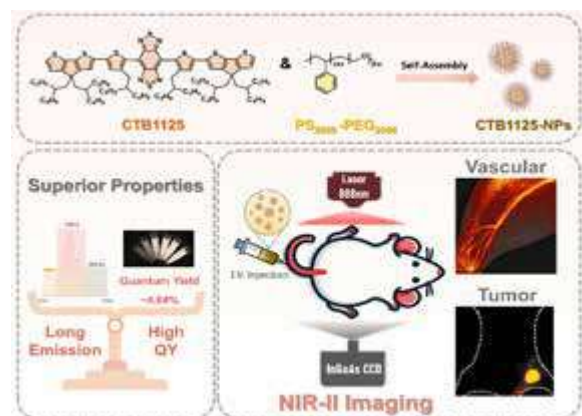
^aShaanxi Normal University.

*Corresponding author: yltang@snnu.edu.cn

Abstract

Focusing on the limited sensitivity of detection and optical imaging, the low therapeutic efficiency and other key issues in diagnosis and treatment of diseases, we have designed and synthesized a series of conjugated polymers fluorescent probes in recent years. Utilizing the excellent fluorescence properties of these probes, we have developed novel methods for highly selective, sensitive, and ultra-fast imaging and sensing of disease biomarkers. We have also designed and synthesized NIR-II probes with high fluorescence quantum yields, as well as novel phototheranostic probes integrating NIR-II imaging and Type-I photodynamic therapy (PDT)/photothermal therapy (PTT), achieving highly sensitive in vivo imaging and efficient theranostics. Furthermore, to address issues such as limited tissue penetration depth of excitation light and background fluorescence interference from biological tissues, we have designed and synthesized chemiluminescent conjugated polymer probes. By taking advantage of the intramolecular chemiluminescence resonance energy transfer (CRET) mechanism, we have realized highly sensitive deep-tissue chemiluminescence imaging for inflammation and tumors, and further achieved efficient excitation-light-free photodynamic anti-tumor therapy. Also, we designed a series of unimolecular chemiluminescent probes using an electron donor engineering strategy. We successfully synthesized the unimolecular probe TTBL, which exhibits NIR-I emission, and the chemiluminescent probe FTBL with an ultra-high quantum yield, enabling highly sensitive chemiluminescence imaging in mouse models of peritonitis and colitis. Additionally, by virtue of the combined CRET and FRET mechanisms, we designed and synthesized a NIR-II chemiluminescent nanosensor, achieving highly sensitive imaging of deep-tissue diseases. Our researches provide new materials and insights for bioimaging and therapy.

Keywords: organic molecular probe, near infrared probe, chemiluminescent probe, imaging, therapy



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ENHANCING FORENSIC ANALYSIS: THE ROLE OF NIR (NEAR- INFRARED) TECHNOLOGY IN ILLICIT DRUG ANALYSIS IN NARCOTICS DIVISON, KIMIA MALAYSIA

Saravana Jayaram^{a*}

Narcotics Division, Kimia Malaysia.

**Corresponding author: saravana@kimia.gov.my*

Abstract

Near-infrared (NIR) spectroscopy has emerged as a powerful, non-destructive and rapid analytical technique for the detection and characterization of illicit drugs. Its ability to provide molecular information without requiring complex sample preparation makes it highly suitable for forensic analysis. NIR operates in the 780-2500 nm range, allowing the identification of chemical compounds based on their unique vibrational overtones and combination bands. One of the key advantages of NIR technology in illicit drug analysis is its capability for in situ and portable field applications. Handheld NIR spectrometers enable forensic chemists to conduct on the spot drug screening, reducing the need time-consuming laboratory analysis. Additionally, NIR can be used to quantify drug purity, distinguish between similar substances and detect adulterants or cutting agents. Despite its advantages, NIR spectroscopy faces challenges such as spectral overlap in complex mixtures and limitations in detecting trace amounts of drugs. However, ongoing advancements in instrumentation, artificial intelligence and data processing techniques continue to improve their sensitivity and specificity.

In conclusion, NIR spectroscopy plays a crucial role in illicit drug analysis due to its speed, non-invasiveness and portability. With continued advancements, it holds great promise for real-time drug detection and forensic investigations, aiding in the fight against drug trafficking abuse.

Keywords: NIR, spectroscopy, drugs, analysis

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SEPARATION AND QUANTITATION OF SACCHARIDE COMPOUNDS IN PERSONAL CARE PRODUCTS USING LIQUID CHROMATOGRAPHY REFRACTIVE INDEX DETECTOR (LC-RID)

Chung Lee Yee^a, Norsyariza. Abd Aziz^a, T.T.C. Ting^a, Hon Yeong Ng^a,
Khan Loon Ng^{a,*}, Mong Sah Toh^a

^aWinnox Cosmeceutics Sdn Bhd. R&D, Subang Jaya, Malaysia.

*Corresponding author: ng.khanloon@wipro-unza.com

Abstract

Biopolymers are increasingly used in the personal care industry for their eco-friendly, biodegradable, and skin-friendly properties. They enhance formulation stability, provide hydration, and moisturizing benefits. The analysis of free sugars in biopolymer is crucial in these products, as they can undergo the Maillard's reaction, leading to undesirable browning and the formation of potentially harmful compounds like furfural. Monitoring this free sugar can ensure stability, safety, and quality of personal care products that prevent negative effects on both product performance and consumer health. In this study we have developed and validated a method for the quantification of free sugars molecules including sugar alcohol using a high-performance liquid chromatography refractive index detector (HPLC-RID). Sugars were separated on sugar specific column with an oven temperature of 80 °C, using an isocratic solvent system of 100% water at 0.5 mL/min flow rate with RID. A total of eight sugar molecules including trehalose, glucose, xylose, galactose, fucose, fructose, ribose, and sorbitol were successfully determined simultaneously. The method showed an acceptable limit of quantification (3.75 µg mL⁻¹) and a calibration curve with a correlation coefficient of above 0.999, covering a concentration range of 62.5 µg mL⁻¹ to 500 µg mL⁻¹ for all sugar molecules. To assure the method reliability, spike analysis of glucose and trehalose on market samples were performed, a good recovery of above 95% was achieved. These attributes shown the method meet the intended application in quality control purpose.

Keywords: sugar profile, biopolymer, HPLC-RID,

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DETERMINATION OF IN-VITRO WATER RESISTANCE RETENTION OF SUNSCREEN PRODUCT

Norsyariza Abd Aziz ^a, Rafiq Farhat Abdul Razak^a, Khan Loon Ng ^{a*}, Mong Sah Toh ^a,

^a Winnox Cosmeceutics, No 7 Persiaran Subang Permai, Taman Perindustrian Subang, 47610 Selangor, Malaysia

*Corresponding author: ng.khanloon@wipro-unza.com

Abstract

Ultraviolet (UV) radiation is the primary cause of various skin diseases, necessitating the need for UV protection¹. People have various sun-protection options to choose including seeking shade, wearing clothes that block the sun and the use of sunscreen product². Topical sunscreens are the commonly used method to achieve this. The good sunscreen formulation should have the ability in keeping the filtration capacity as long as possible after being applied to the skin and capable of fixing themselves at the level of the superficial layers of the epidermis without penetrating deeply into the skin³. This substantivity is closely linked to the water resistance properties⁴. Currently the water resistance retention (WRR) of sunscreen formulation based on in-vivo method carried out on healthy human subjects as according to Colipa method. This method is very restrictive and poses an ethical problem since the subjects are exposed to radiation. In this study, a simple reproducible and reliable in-vitro method was developed for evaluation of the WRR of sunscreen products based on polymethyl methacrylate (PMMA) plate as the substrate. The in-vitro sun protection factor (SPF) of the sunscreen formulation was evaluated at initial condition and after 40 minutes immersion in water bath in coloration with a specific biological action spectrum and relevant sun emission spectrum. The percentage of WRR for sunscreen products calculated based on the in-vitro SPF value after 40 minutes of water immersion against initial in-vitro SPF value. The water resistance claim of sunscreen formulation is valid only for formulation having the percentage WRR more than 50%. The method was validated based on the reference sunscreen formulation as per recommended by Colipa method and in compliance with ISO 24444:2019, FDA 2011 and ISO 24442:2022. The method was successfully applied for assessment of WRR of in-house formulations and market samples.

Keywords: In-Vitro SPF, Water Resistant Retention

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AUTOMATIC BIOSENSING VIA DIGITAL MICROFLUIDICS COMBINED WITH CHEMILUMINESCENCE

Yan Jin^{a,*}, Hairensa Maimaitiyili^a

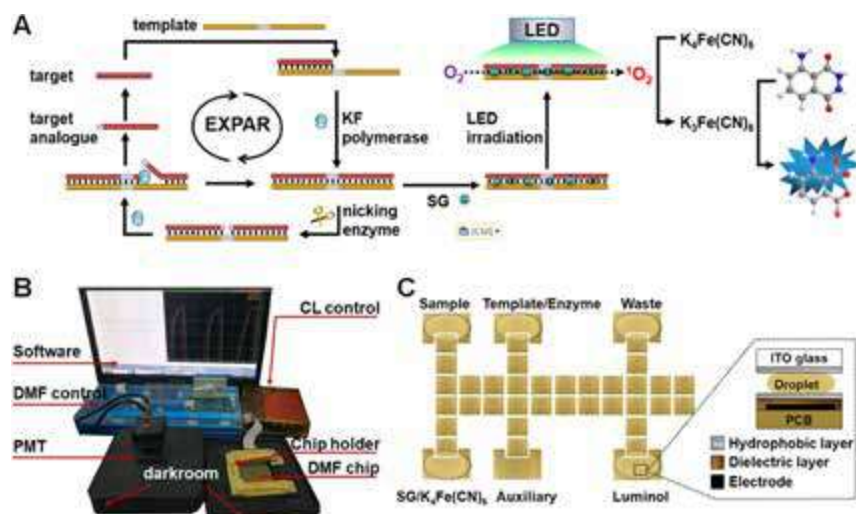
^aShaanxi Normal University

*Corresponding author: jinyan@snnu.edu.cn

Abstract

Digital microfluidics (DMF) is an emerging microfluidic technology to automatically manipulate discrete droplets for mixing, reaction and splitting, etc. Due to the advantages of simple equipment, high sensitivity and rapid detection, chemiluminescence (CL) technique holds advantages to integrate with DMF for automatic and sensitive bioassay. Recently, our group constructed a DMF-CL integration device to achieve automated bioanalysis. The reliability and stability of droplet manipulation were investigated through droplet movement, splitting, mixing and intracellular nucleic acid extraction. A novel droplet splitting method, called asymmetric splitting, was proposed to address the shortcomings of current droplet splitting methods. The CL behavior of a new glow-type CL reaction was investigated in situ and online by using DMF-CL. Copper-cysteine nanoparticles with peroxidase-like activity catalyzed the luminol- H_2O_2 reaction, which extended to ten minutes. Comparison with the results of conventional CL analyzer indicated that the DMF-CL platform could intelligently and reliably study the kinetics of CL reactions¹. Moreover, a DMF-CL method based on isothermal exponential amplification was constructed for sensitive detection of human immunodeficiency virus DNA without the need of a complicated thermal cyclers.² These explorations demonstrated that DMF-CL holds a great potential for diverse and automatic biosensing.

Keywords: digital microfluidic, chemiluminescence, automatic biosensing, DNA, chemiluminescence kinetics



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NANOCRYSTALLINE CELLULOSE HYDROGEL ENCAPSULATED PLASMONIC NANOSENSORS FOR DETECTION OF REACTIVE OXYGEN SPECIES (ROS): TOWARDS A SENSING BANDAGE

Yusra Rabbani^{a,*}; Idriss Blakey^{a,b}; Yuan Xu^c; Jason Stokes^c; Paul Denman^a,

^a*Australian Institute for Bioengineering & Nanotechnology, The University of Queensland, Australia.*

^b*Centre for Advanced Imaging, The University of Queensland, Australia.*

^c*School of Chemical Engineering, Faculty of Engineering, Architecture and Information Technology, The University of Queensland, Australia.*

**Corresponding author: y.rabbani@uq.edu.au*

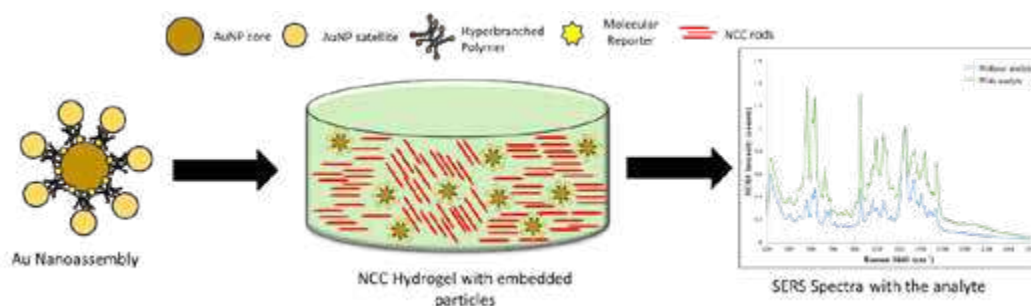
Abstract

Chronic wounds cause a socioeconomic strain upon the healthcare system. These are consequences of diseases such as diabetic foot ulcers or burns. Healing of such wounds can be delayed due to the presence of excess Reactive Oxygen Species (ROS), mainly hydrogen peroxide. Treatment using ROS modulation could increase the potential for optimizing the healing process and reducing healthcare costs.

This seminar describes embedding plasmonic sensors into hydrogels that can be incorporated into bandages with an aim to ultimately allow non-invasive monitoring of ROS concentrations at wound sites using Surface Enhanced Raman Spectroscopy (SERS). The plasmonic nanosensors are discrete core-satellite nanoassemblies of gold nanoparticles which are linked with hyperbranched polymers (HBP). The HBPs create a sub 10 nm gap that results in the SERS enhancements. These nanoassemblies are then embedded into Nanocellulose Crystal (NCC) hydrogels. NCCs gels have a complex phase diagram ranging from ordered liquid crystals to anisotropic gels where viscoelastic properties are strongly phase dependent.

A specific aim of this study was to examine the factors that impact the arrangement of the plasmonic sensors in the different phases of NCC gels, as well as how the phases influence diffusion profiles of the analyte, as these factors play a significant role in dictating the performance of the composites as sensing materials. In this way the study will offer key insight for designing novel SERS-based hydrogel nanosensor for development of smart bandages that allow non-invasive detection and monitoring of ROS at chronic wounds.

Keywords: Sensors, Gold nanoparticles, SERS, NCC,



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TOTAL-REFLECTION X-RAY FLUORESCENCE (TXRF) AS A PROMISING METHOD FOR GEOCHEMICAL RESEARCHES

Artem Maltsev^{a*}, Alena Zhilicheva^a, Galina Pashkova^a, Alexei Ivanov^a

^a*Institute of the Earth's Crust, SB RAS, Russia*

*Corresponding author: artemmaltsev1@gmail.com

Abstract

Total reflection X-ray fluorescence (TXRF) is currently one of the few analytical methods that provide rapid and cost-effective multi-element analysis of various liquid and solid samples. The main advantages of TXRF are as follows:

- small sample volume (μL-mL or μg-mg range);
- variety of sample preparation procedures (direct analysis, acid digestion, preconcentration or extraction);
- quantification by internal standard method (no external calibration required);
- rapid screening (semi-quantitative and quantitative multi-element analysis within 200-1000 s);
- low operating costs.

The above advantages of TXRF indicate the prospects of TXRF compared to other atomic spectroscopy methods such as AAS, AES or ICP-MS, which are commonly used for geochemical studies. The report presents our laboratory's experience in using TXRF spectrometry for elemental analysis of apatite, fluorite, nodules and ores. [1-4]. Particular attention is paid to the sample preparation procedure, since it is one of the main sources of measurement errors. One of the methodological issues is the difficulty of preparing a thin, homogeneous sample from a solid sample with a complex mineral matrix. The sample preparation strategy should be selected taking into account the characteristics of the sample, the content of the elements being determined, and the accuracy required for reliable interpretation. Examples of preparing a suspension for express analysis of ores and nodules, original methods of chemical decomposition of apatite and fluorite are considered. The presented methods are successfully applied for geochemical exploration.

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Keywords: TXRF, figures of merit, method development, sample preparation, quantification

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BRIDGING ANALYTICAL METHODS AND PRACTICAL SOLUTIONS: ACCURATE QUANTIFICATION OF SILOXANES AND SULFUR IN BIOGAS

**Ayush Agarwal^{a,b,*}, Laura Torrent^{a,c}, Julian Indlekofer^a, Sylvain Bouchet^d, Lucy P. Culleton^e,
Serge M.A. Biollaz^a, Christian Ludwig^{a,b}**

^aPaul Scherrer Institute, PSI Center for Energy and Environmental Sciences, 5232 Villigen PSI, Switzerland.

^bÉcole Polytechnique Fédérale de Lausanne (EPFL), School of Architecture, Civil and Environmental Engineering (ENAC IIE GR-LUD), 1015 Lausanne, Switzerland.

^cUniversity of Girona (UdG), Department of Chemistry, Faculty of Sciences, 17003 Girona, Spain.

^dFederal Institute of Metrology, METAS, Lindenweg 50, CH-3003 Bern-Wabern, Switzerland.

^eNational Physical Laboratory (NPL), Hampton Road, Teddington, Middlesex, UK, TW11 0LW

*Corresponding author: ayush.agarwal@epfl.ch

Abstract

Biogas, an increasingly important renewable energy source, faces operational challenges due to trace contaminants such as siloxanes and sulfur compounds. These impurities, even at low concentrations, contribute to catalyst poisoning, corrosion, and mechanical degradation, thereby reducing overall system efficiency and longevity. Consequently, accurate and reliable quantification methods for these contaminants are crucial for effective monitoring and optimal biogas utilization.¹

The primary objective of this study was to develop and validate a simplified yet robust analytical method capable of simultaneously quantifying siloxanes and sulfur compounds in biogas. Emphasis was placed on accuracy, precision, ease of sample handling, and applicability to practical scenarios across small- to medium-scale biogas plants.

We employed a liquid quench (LQ) sampling technique combined with gas chromatography-inductively coupled plasma mass spectrometry (GC-ICP-MS). The method utilizes liquid calibration standards instead of traditional gaseous standards, thereby significantly simplifying calibration procedures. To validate reliability and reproducibility, the developed analytical procedure was tested through participation in a comprehensive round robin test. Sample stability was assessed over storage periods up to four weeks to confirm analyte preservation.

The analytical approach demonstrated high accuracy and reproducibility, validated through inter-laboratory comparison and robust performance across various biogas plants in Switzerland. The method's use of liquid calibration standards minimized errors commonly associated with gaseous standard-based calibration. Additionally, analytes showed negligible degradation during extended storage periods, affirming the suitability of this approach for routine operational monitoring.

This study presents a validated and practical method enabling simultaneous quantification of siloxanes and sulfur compounds in biogas. By simplifying sampling and calibration, it facilitates broader implementation in biogas facilities lacking advanced analytical infrastructures. Ultimately, the method enhances impurity monitoring, contributing significantly to improved biogas quality management and optimized renewable energy production.

Keywords: Siloxanes; Sulfur Compounds; Bioenergy; Trace impurities; Gas metrology

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ELUCIDATING THE IMPACT OF FEED SOURCES AND ADULTERATION ON STINGLESS BEE HONEY QUALITY AND TOXICITY

Farah Adilah Md Jafry^a, Rabiatal Adawiah Mohd Noor^a, Siti Munirah Mohd Faudzi^b, Syahida Ahmad^b, Norhasnida Zawawi^{c*},

^aLaboratory of Halal Services, Halal Products Research Institute, Universiti Putra Malaysia

^bNatural Medicines and Products Research Laboratory, Institute of Bioscience, Universiti Putra Malaysia

^cDepartment of Biochemistry, Faculty of Biotechnology and Science Biomolecules, Universiti Putra Malaysia

*Corresponding author: norhasnida@upm.edu.my

Abstract

The high market value of stingless bee honey (SBH) attracts unethical adulteration, including indirect adulteration, which may pose health concerns. A study has been conducted by Hungerford et al. (2021) to study the effect of sucrose direct feeding on the quality of stingless bee honey. Still, no studies have been undertaken to study the impact on Malaysian SBH. Therefore, this study investigates the effect of feed sources – naturally fed SBH (H) and indirect adulteration (AH) with sucrose or floral nectar solution (FNS) on SBH quality and toxicity. The primary variables that were further studied were the differences in honey quality between naturally fed (H) bees from multifloral and *Cocos nucifera* farms, compared with direct feeding (AH) of either sucrose solution or *C. nucifera*, using the *Heterotrigona itama* (1) and *Geniotrigona thoracica* (2) bee species. The physicochemical and antioxidant properties were determined using HPLC-ELSD and LC-MS-QTOF. An acute toxicity study was conducted on brine shrimp and adult zebrafish. Results show that *C. nucifera* FNS contains sucrose (0.56 ± 0.01 g/100 g), Total Phenolic Content (2.151 ± 0.017 mg GAE/g), Total Flavonoid Content (0.131 ± 0.039 mg QE/g), and Ferric-Reducing Antioxidant Power (5.588 ± 0.173 mg FeSO₄/g), compared to the sucrose solution. The effects of feed sources on the physicochemical and antioxidant properties of H and AH were inconsistent, as shown by the species-specific variations of AH with *G. thoracica*, which exhibited higher trehalulose levels (59.82–84.78 g/100 g) compared to AH from *H. itama* (53.83–67.06 g/100 g). Higher antioxidant properties were also observed in AH from *H. itama* (TPC: 331.66 - 512.45 µgGAE/g; TFC: 32.40 - 70.31 µgQE/g; FRAP: 102.54 - 300.91 µgFeSO₄/g) compared to AH from *G. thoracica* (TPC: 179.14 - 385.39 µgGAE/g; TFC: 26.63 - 53.52 µgQE/g; FRAP: 30.72 - 328.54 µgFeSO₄/g). Nevertheless, all AH honey contains fewer chemical compounds when analysed using LCMS. Some chemical markers indicative of sucrose feeding were also identified. Additionally, all AH honey samples were observed to induce mild toxicity at a 5 mg/g bw concentration, with a 72.73–90.91% survival rate compared to H honey. In conclusion, these findings underscore the substantial impact of bee species and feed sources on the quality and safety status of SBH. The data can be used by governing bodies to determine the quality and safety of stingless bee honey sold in the market.

Keywords: stingless bee honey, physicochemical, adulteration, quality, safety

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STRUCTURE LIPIDOMICS – LARGE SCALE, IMAGING AND SINGLE CELL ANALYSIS

Zheng Ouyang^{a,*}, Xiaoxiao Ma^a, Wenpeng Zhang^a, Yu Xia^a

^aTsinghua University, Beijing 100084, China

*Corresponding author: ouyang@tsinghua.edu.cn

Abstract

Structural lipidomics has emerged as a powerful approach for obtaining high-definition lipidome data, enabling the annotation of lipid species with high specificity and detailed structural resolution.^{1, 2} To achieve this, we developed a method combining photochemical derivatization with tandem mass spectrometry (MS/MS) to identify critical structural features, including C=C double bond locations, sn-positions, and other lipid modifications. This strategy has been successfully applied in large-scale lipidomics studies using LC-MS/MS, resolving hundreds of lipid species in extracts from bovine liver samples.

However, applying this approach to tissue imaging and single-cell lipidomics has been challenging due to the limitations of conventional MS/MS methods, which struggle with small sample volumes. To overcome this, we developed novel strategies to significantly improve MS/MS analysis efficiency for samples desorbed during imaging or extracted from single cells.

One approach employs a dual linear ion trap (LIT) configuration, where ions are first trapped in one LIT and then mass-selectively transferred to a second LIT for sequential MS/MS analysis.³ Another method utilizes a Cyclic instrument, leveraging ion mobility to modulate ion mixture composition.⁴ Here, ions across wide *m/z* ranges are sequentially analyzed via quadrupole-TOF MS/MS, followed by spectral deconvolution to reconstruct MS/MS spectra. Additionally, we incorporated spatial lipid distribution data from tissue imaging to aid in MS/MS deconvolution, enabling the analysis of tens to over 100 lipid species in imaging and single-cell applications.

Further advancements include on-tissue and on-cell photochemical derivatization, allowing precise localization of C=C bonds, and MS³ analysis of sodiated lipid ions for resolving sn-positions.⁵ These innovations collectively enhance structural lipidomics at the microscale, opening new avenues for spatial and single-cell lipidome profiling.

Keywords: Structural lipidomics, photochemical derivatization, tissue imaging, single cell analysis

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COMMON MINERALS DISINTEGRATE IN MICRODROPLETS FORMING NANOPARTICLES (A PATH TO SUSTAINABLE AGRICULTURE)

Thalappil Pradeep

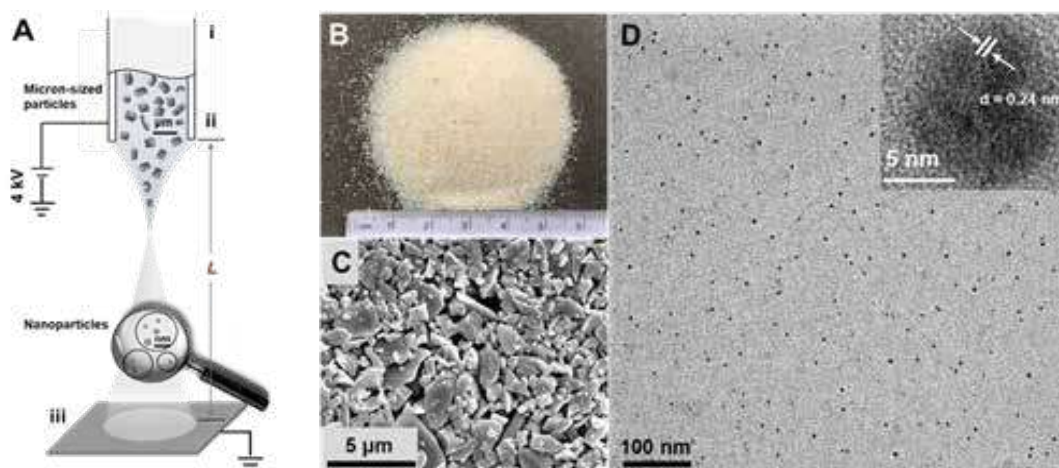
Indian Institute of Technology Madras, Chennai, 600 036, India

**Corresponding author: pradeep@iitm.ac.in*

Abstract

Soil is formed from rocks, textbooks say. It is a slow process; one cm thick soil takes 200-400 years to form depending on conditions. Nanoscale particles are most essential constituents of soil which help in plant growth. We showed that common mineral particles break down spontaneously to form nanoparticles within milliseconds when encapsulated in charged water microdroplets. In our experiments, micrometer-sized minerals such as quartz and ruby were transformed into nanoparticles ranging from 5 to 10 nanometers. Computer simulations helped us to understand the process. This rapid weathering process could significantly contribute to soil formation, considering the widespread presence of charged aerosols in the atmosphere. The process could also be used to make soil industrially, to enhance agricultural productivity. The active surfaces of materials formed in microdroplets could lead to catalysis of relevance contributing to the biological evolution of the planet.

Keywords: Analytical Chemistry, Microdroplets, Electrospray, Nanomaterials, Sustainable chemistry



(A) Electro-spray of a water suspension of micro-scale mineral particles at 4 kV resulting in charged microdroplets on a substrate held at a varying distance (L) to make nanoparticles. (B) Parent natural silica (sand), (C) micron-sized particles of silica used for electro-spray and (D) resulting nanoparticles of silica with an individual particle shown in the inset. (From Ref. 3)

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PUSHING THE BOUNDARIES OF LIPIDOMIC PROFILING TOWARD LOW-ABUNDANCE LIPID CLASSES

Yu Xia*

^a Department of Chemistry, Tsinghua University, Beijing, China

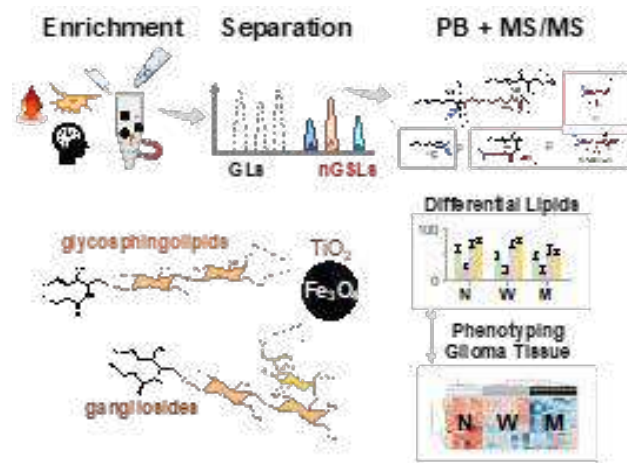
*Corresponding author: xiayu@tsinghua.edu.cn

Abstract

The lipidome consists of thousands of distinct lipid species, with concentrations spanning at least eight orders of magnitude. However, low abundance lipid classes, which typically constitute less than 1% of total lipid mass, stand outside the dynamic range allowed from conventional lipidomic analysis workflows. Herein, we have developed selective enrichment methods for neutral glycosphingolipids (nGSL) and gangliosides, respectively, using magnetic titanium dioxide nanoparticles (TiO₂ MNPs).^{1,2} These methods rely on forming strong coordination between the cis-diol of the glycan headgroup with Ti (IV) under basic pH conditions. Under these conditions, the interfering phospholipids only form weak electronic interactions with Ti (IV) which can be subsequently removed by washing buffer containing ammonium salt. These methods allow 30- to 100-fold enrichment of nGSLs and gangliosides from lipid extracts, achieving detection limits in the sub-nM range. By combining selective enrichment with charge-tagging Paternò-Büchi reaction, and liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis, we identify over 600 distinct structures of nGSLs and gangliosides from porcine brain lipid extract and human plasma at multiple structural levels, including subclass, species, chain composition, and double bond location. These deep-profiling workflows also reveal dysregulated metabolism of nGSLs and gangliosides in human glioma tissue and breast cancer cells.

Keywords:

glycosphingolipids, gangliosides, magnetic titanium dioxide nanoparticles, lipid isomers, the Paternò-Büchi reaction



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ANALYSIS OF VOLATILE ORGANIC COMPOUNDS (VOC) IN SELECTED COOKING OILS USING HEADSPACE-GC/MS TECHNIQUE

Raznim Arni Abd. Razak^{1*} and Azmil Haizam Ahmad Tarmizi¹

¹*Product Development & Advisory Division, Malaysian Palm Oil Board, 6, Persiaran Institusi, Bandar Baru Bangi, 43000 Kajang, Selangor, Malaysia*

**Corresponding author: raznim@mpob.gov.my*

Abstract

Volatile organic compounds (VOC) are generally formed during frying due to the high temperatures and chemical reactions occurring in cooking oils. These compounds could affect human health related to respiratory irritation and indoor air quality. Harmful VOC typically are not toxic (acute), but VOC such as 1,3-butadiene, benzene, formaldehyde and acrolein are known to have carcinogenicity effect to human. This study was designed to develop headspace-GC/MS method for the detection and identification of VOC in cooking oils during heating. The headspace-GC/MS method was successfully developed by heating the related cooking oils at different headspace incubation temperatures and times. Analysis of VOC using headspace-GC/MS revealed the presence of six compounds in the oils namely hexanal, heptanal, pentanal, octane, 2,4-heptadienal and trans-2-octenal. The results also indicated the increment of VOC formation, which is proportional with higher headspace temperatures and longer heating times. Palm olein exhibited lower VOC formation, while corn, sunflower, and high oleic sunflower oils exhibited significantly higher VOC release. Pearson correlation analysis showed that heating the oils at 180 °C displayed a strong and positive correlation between VOC and alterations in monounsaturated fatty acids (MUFA), but gave moderate negative correlation with changes in saturated fatty acids (SFA), polyunsaturated fatty acids (PUFA), and trans-fatty acids (TFA).

Keywords: Volatile organic compounds; Heating; Headspace-GC/MS; Cooking oils; Fatty acids

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APPLICATIONS OF ISOTOPE RATIO MASS SPECTROMETRY (IRMS) TO FORENSIC SCIENCES

Lionnel Mounier

Thermo Fisher Scientific, 16 avenue du Québec SILIC 765 Villebon-sur-Yvette 91963 Coutaboeuf Cedex France

**Corresponding author: lionnel.mounier@thermofisher.com*

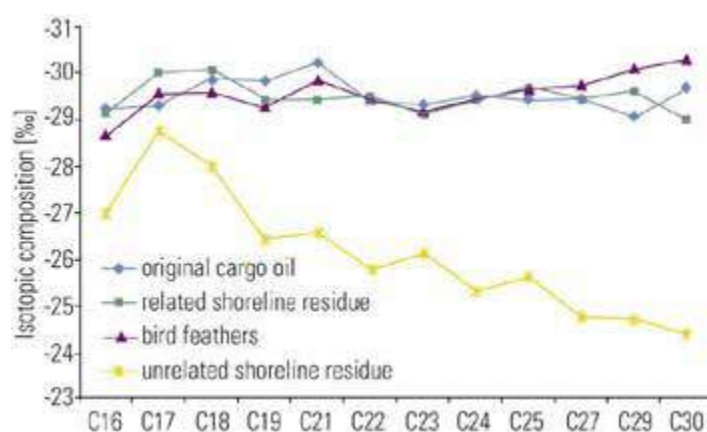
Abstract

As the name indicates, isotope ratio mass spectrometry (IRMS) is an analytical technique that measures the subtle variations in the ratios of isotopes. The technique is applicable to most of the periodic table. These mass spectrometers make use of a magnetic sector analyzer that deflects at different angles different isotopic ions produced in a variety of ion sources and collects them with a multi-collector detector. One of the earliest versions of mass spectrometry was developed in the early 1920s, although it did not become a commercialized technology until the late 1940s.

IRMS is a technique which finds its initial application developments in geosciences and in nuclear sciences. The introduction of new commercially available relatively high sample throughput instrumentation such as Multi-Collector Inductively Coupled Plasma Mass Spectrometry (MC-ICP-MS) and Continuous Flow Stable Isotope Ratio Mass Spectrometry (CF- SIRS) generated a significant growth in the number of users and in the variety of applications since two or three decades.

The application of isotope fingerprints to forensic investigations has become more commonplace because there is a need for a rigorous scientific foundation underpinned by sound analytical techniques. IRMS can provide a unique insight into the origin or production of a diversity of materials such as drugs or explosives. In criminology, it can help tracking human geographical origin or establishing unknown's identity as well as linking or separating remains. IRMS also help to correlate between drug seizures and pollutants to polluters. The technique is moreover used for nuclear forensics investigations.

Keywords: forensic sciences, isotope fingerprinting, isotopic ratio mass spectrometry



Example of environmental forensic: relating oil spills to their origin

HPLC METHOD FOR THE SIMULTANEOUS DETERMINATION OF SUGARS AND MEDIUM-CHAIN CARBOXYLIC ACIDS IN MICROBIAL FERMENTATION SAMPLES

**Liyana Salwa Mohd Nazir^{a*}, Siti Amira Mat Hussin^a,
Fatin Nur Amira M Hejemi^a, Voon Chang Hong^a**

^aPETRONAS Research Sdn. Bhd, Jalan Ayer Itam, Kawasan Institusi Bangi, 43000 Kajang, Selangor.

** Corresponding author: liyana_salwa@petronas.com*

Abstract

Medium-chain carboxylic acids can be produced through microbial chain elongation processes that utilize sugars such as fructose as a carbon source. Typically, carboxylic acid analysis is conducted using gas chromatography (GC), while sugar analysis is performed using high-performance liquid chromatography (HPLC). In this study, an analytical method was developed using high-performance liquid chromatography with refractive index detection (HPLC-RID) for the simultaneous identification and quantification of sugars and short-to medium-chain carboxylic acids in aqueous fermentation samples. The target analytes included glucose, sucrose, fructose, acetic acid, propionic acid, butyric acid, valeric acid, hexanoic acid, and 2-ethylhexanoic acid. Separation was achieved using a Hi-Plex H ion-exclusion column at 30 °C, with 0.005 M sulfuric acid as the mobile phase at a flow rate of 0.6 mL/min. The column effluent was monitored using a refractive index detector. This method was validated in terms of selectivity, linearity, precision, accuracy, limit of detection and limit of quantification. This method allows for the simultaneous analysis of sugars and carboxylic acids in a single run and is applicable for monitoring microbial fermentation processes.

Keywords: HPLC-RID, Medium-chain carboxylic acid, ion exclusion chromatography, organic acid, sugars

DETERMINATION OF HEXAMETHYLENETETRAMINE IN STRONGLY ACIDIC INDUSTRIAL PICKLING SOLUTIONS BY CAPILLARY ZONE ELECTROPHORESIS

Botas C^{a,*}, Moreno-Barambio M^b, Dominguez C^a, Martinez G^a, Sanchez-Arribas A^b

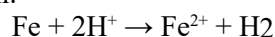
^aArcelorMittal Global R&D

^bDto de Química Analítica y Análisis Instrumental. Universidad Autónoma de Madrid, Spain

*Corresponding author: cristina.botas@arcelormittal.com

Abstract

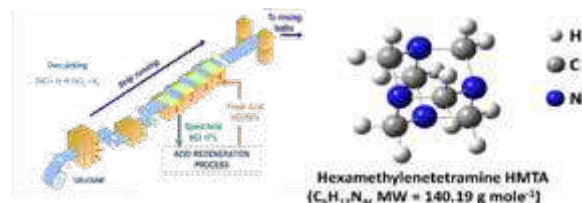
In the industrial production of flat carbon steel, strip is covered by scale after hot rolling step, an oxide layer a few microns in thick. To remove this layer, the steel strip is pickled by immersion into the baths containing a concentrated hydrochloric (HCl) or sulphuric aqueous acid solution. The reaction products are iron cations and water. Iron cations can further combine with chloride or sulphate ions. When the scale is eliminated from the steel surface, protons also react with the base steel following the reaction:



The production of hydrogen gas is characteristic of the corrosion of base steel. To prevent it a corrosion inhibitor is added to the pickling bath. Amines present significant inhibitive efficiency thanks to the electronegativity of their nitrogen atoms. An amine typically used in commercial inhibitor solutions for pickling baths is hexamethylenetetramine (HMTA, IUPAC name 1,3,5,7-tetraazatricyclo[3.3.1.1(3,7)]-decane).¹

Although HMTA use is widespread in the steel industry, it is difficult to find methods for its determination in the literature. Accurate monitoring of HMTA is essential to ensure optimal performance, process control, to adjust the required HMTA amount, and compliance with environmental standards. This study presents the development of a capillary zone electrophoresis (CZE) method for its determination.

The method has been designed to overcome the challenges associated with analysing samples from strongly acidic media (pH < 1), with high ionic strength and significant metal content (>100 g/L), typical of this industrial process. The proposed CZE method enables simple and fast quantification of HMTA. The simplicity and fast turnaround of this methodology make it a practical and efficient tool for the routine monitoring of HMTA in industrial samples. The results obtained in this study confirm the degradation of the compound in samples of different natures from the industrial pickling process.



Keywords: Hexamethylenetetramine, Capillary Electrophoresis, Over-Pickling inhibitor, steelmaking

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APPLICATION OF LC-MS-BASED METABOLOMICS IN OPTIMIZING HARVESTING TIME AND PLANT PART SELECTION IN *BAECKEA FRUTESCENS*

Fauziah Abdullah*¹, Adiana Mohamed Adib¹, Hada Masayu Ismail@Dahlan², Zunoliza Abdullah¹,
Fadzureena Jamaludin², Nursabrina Najwa Salmin¹, Mohamad Nazrin Che Saad¹ and Hafidz Hadi
Abdullah¹

¹Herbal Quality Control Programme, ²Bioresources Programme, Natural Products Division,
Forest Research Institute Malaysia, 52109 Kepong, Selangor

*Corresponding author: fauziahabdullah@frim.gov.my

Abstract

Baeckea frutescens (Myrtaceae) is a medicinal plant traditionally used to treat inflammation-related conditions, with reported high in xanthine oxidase inhibitory activity. Previous studies identified 6-methylquercetin as a key bioactive compound, primarily concentrated in the stem. HPLC-based quantification from our earlier work suggested that harvesting between 12 and 18 months yielded the highest concentration of this metabolite. In this study, untargeted LC-MS-based metabolomics was employed to investigate metabolic differences between the leaves and stems of *B. frutescens* at various growth stages. MS/MS fragmentation data were analyzed using the *in-silico* annotation platform SIRIUS, resulting in the tentative identification of more than 40 metabolites. Partial Least Squares Discriminant Analysis (PLS-DA) revealed a clear separation between the two plant parts based on their metabolite profiles, indicating a distinct part-dependent metabolic composition. Variable Importance in Projection (VIP) analysis identified several key discriminant metabolites with VIP scores >1.5, including 6-methylquercetin, ursolic acid, and quercetin-3-*O*-rhamnoside. These compounds were more abundant in the stem, as shown in the loading plots, and heatmap analysis indicated that their levels peaked at 18 months. These findings supported earlier HPLC-based results and further highlighted additional metabolite markers valuable for determining optimal plant parts and harvesting times. Overall, this study demonstrates that LC-MS-based metabolomics provides a robust platform for profiling the metabolic composition of *B. frutescens*, supporting the 18-month-old stem as the most suitable source for bioactive extract standardization and herbal product development.

Keywords: *Baeckea frutescens*, LC-MS based metabolomics, harvesting time, multivariate data analysis.

SURFACE CHEMISTRY AND TRIBOLOGY IN ACTION: BRIDGING MATERIAL DESIGN AND PERFORMANCE

Damien Yiyuan Khoo

Bruker Nano Inc, 101 Daggett Drive, San Jose, CA 95134, USA.

**Corresponding author: damien.khoo@bruker.com*

Abstract

The interface between surfaces in relative motion is a critical zone where material design, surface chemistry, and mechanical forces intersect to dictate tribological performance. Surface chemistry plays a critical yet often underappreciated role in governing tribological performance. From friction and wear behavior to lubrication effectiveness, the interactions at material interfaces are shaped not only by mechanical loading but also by the chemical composition, structure, and reactivity of surfaces in contact. This presentation explores how surface chemistry can be engineered and characterized to bridge the gap between material design and tribological performance, with a focus on practical applications in automotive, manufacturing, and precision engineering. The talk highlights key mechanisms by which surface chemistry influences tribological behavior—such as tribofilm formation, interfacial adhesion, and chemical wear. Case studies will illustrate how chemical modifications (e.g., coatings, surface functionalization, and additives) can enhance wear resistance and reduce friction in both dry and lubricated systems. Special emphasis is placed on polymer-metal interfaces, nanocomposite coatings, and chemically active lubricant formulations. A range of advanced surface characterization techniques will be discussed for their ability to analyze surface composition, chemical states, and morphological changes at the micro- and nanoscale. These methods are essential in correlating surface chemistry with tribological outcomes and guiding material optimization. By integrating insights from surface chemistry into the design process, engineers and materials scientists can develop application-specific solutions that improve performance, extend component life, and reduce energy losses. This presentation offers a multidisciplinary perspective on how to leverage chemical and tribological principles together to design next-generation materials and surfaces tailored to demanding operational environments.

Keywords: Surface chemistry, tribology, friction, wear, material design.

TRACKING FOREVER CHEMICALS USING LCMS AND GCMS: A COMPLEMENTARY APPROACH FOR COMPREHENSIVE DETECTION

Poh Wei Tan^{a*}, Huey Bing Chong^{a*}

^a Agilent Technologies Inc.

* Corresponding author: poh-wei.tan@agilent.com, huey-bing.chong@agilent.com

Abstract

The targeted analysis of Per- and polyfluoroalkyl substances (PFAS) is critical for environmental monitoring, regulatory compliance, and exposure assessment. While liquid chromatography mass spectrometry (LC-MS) has become the primary tool for quantifying ionic and polar PFAS, gas chromatography mass spectrometry (GC-MS) offers unique advantages for detecting volatile and neutral PFAS, such as fluorotelomer alcohols (FTOHs), perfluoroalkyl iodides (PFAIs), and other precursors. This presentation highlights the strength of LC-MS and GC-MS in targeted PFAS analysis, covering method development, sample preparation, matrix considerations, and compound-specific detection challenges. The integration of these techniques enhances analytical coverage and supports a more robust understanding of PFAS presence across environmental and industrial matrices.

Keywords: PFAs Analysis, GCMS, LCMS, Mass Spectrometry, Volatile PFAS

FLUORESCENT CHEMOSENSORS FOR THE SELECTIVE DETECTION OF ORGANIC MOLECULES

Balamurugan Rathinam*

*Department of Chemical and Materials Engineering, National Yunlin University of Science and Technology,
Yunlin-64002, Taiwan, Republic of China. Tel: +886-5-5342601 ext. 4616*

Corresponding author: balar@yuntech.edu.tw

Abstract

The design and development of effective fluorescent probes for the trace recognition of detection of small cations, anions, and neutral molecules in the aqueous, mixed organic aqueous media, environmental specimen, living things e.g., body fluids, serum, urine etc is the evergreen research area. Herein, we report our recently developed fluorescent sensors for the detection of organic molecules such as oxalic acid and ciprofloxacin. Oxalic acid (OA) is occurring in various type of plants, vegetables and microorganism and their concentration in the urine is the primary measurement for renal stone diagnosis^[1-4]. These caused the urgent need to develop a novel strategy for accurate determination of OA content in food as well as wastewater. Therefore, rhodamin-6G based dinuclear zinc complex was designed as a fluorescent probe for the selective detection of OA. Thus designed sensor exhibited rapid fluorescent “turn-on” response along with high selectivity towards OA over other dicarboxylic acids with the detection limit of 1.20 mM at neutral pH. Spectral characterization revealed that the amide from spirolactum ring open-form of the signaling unit (rhodamine) and the zinc complexes are the two binding sites for the selective coordination of OA (Fig. 1). Moreover, we also designed a novel fluorescent receptor based on citrate functionalized zirconium-based metal organic framework (C-MOF-808) for the detection of Ciprofloxacin (CIP), which is a commonly used antibiotic for the treatment of infectious diseases in humans. Thus, synthesized receptor can be used for the fluorescent detection of CIP in aqueous media with a detection limit of 9.4 μM . The development of novel sensor for the detection of another organic molecule namely Cadaverine, which is liberated during the spoilage of meat is under progress.

Keywords: Oxalic acid; Fluorescent Probe; Ciprofloxacin; Metal Organic Framework; Detection limit

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POLYMER-MODIFIED ELECTRODES FOR THE ELECTROANALYSIS OF TRACE METAL IONS AND NITRITES IN WATER AND FOOD SAMPLES

Modou Fall^{a*}, Ismaila Diédhiou^{a,b}, Momath Lô^a, Nouredine Raouafi^b.

^a*Laboratory of Organic Physical Chemistry and Environmental Analyses, Department of Chemistry, Faculty of Sciences and Technics, Cheikh Anta Diop University, Dakar, Senegal.*

^b*Sensors and Biosensors Group, Analytical Chemistry and Electrochemistry Lab (LR99ES15), University of Tunis El Manar, 2092 Tunis El Manar, Tunisia.*

**Corresponding author: modou.fall@ucad.edu.sn*

Abstract

Nitrite and heavy metals ions are can be found in environmental samples such as water, soil, food, and agricultural products. These ions are frequently analyzed to determine pollution levels^{1,2}. In this work, we prepared a poly(sulfanilic acid)-modified glassy carbon electrode (pSA/GCE) by electrochemical polymerization of sulfanilic acid (4-aminobenzenesulphonic acid), and benzene sulfonic acid-doped polypyrrole thin films on aminobenzenediazonium-modified flexible ITO electrodes PPY(BSA)/ITO.

After electrochemical characterization and optimization of the detection parameters, pSA/GCE was used for the determination of nitrite ions by square wave voltammetry (SWV). The electrode was successfully applied to the detection of nitrite ions in salami and ham samples. PPY(BSA)/ITO enabled the simultaneous detection of Cu²⁺, Cd²⁺ and Pb²⁺ by differential pulse voltammetry (DPV).

pSA/GCE was able to detect nitrite over a wide range of concentrations (from 25 µM to 10 mM). A limit of detection of 2.65 µM and a sensitivity of 1.08 µA.µM⁻¹.cm⁻² were obtained. The same electrode was successfully applied to the detection of nitrite ions in salami and ham samples. PPY(BSA)/ITO exhibited excellent electroactivity in the doped state with BSA, which served to chelate the metal ions in aqueous medium. The detection limits were 11.1, 8.95, and 0.99 nM for Cu²⁺, Cd²⁺, and Pb²⁺, respectively. In addition, the modified electrodes displayed good reproducibility, making them suitable for the determination of heavy metals and nitrite in real wastewater samples.

Keywords: Sensing, Nitrite, Heavy metals ions, Surface modification.

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THE EVOLUTION OF MULTIDISCIPLINARY RESEARCH: A JOURNEY OF ANALYTICAL EXCELLENCE AT THE DEPARTMENT OF CHEMISTRY MALAYSIA

Noor Azimah Sulaiman, Farah Idwani Abd. Rahman, Fathiah Ahmad Zubaidi,
Izharudin Che Amat, Wan Farah Nasuha Wan Iskandar

Research and Instrumentation Section, Department of Chemistry Malaysia,

Petaling Jaya, Selangor, Malaysia

Corresponding author: azimah@kimia.gov.my

Abstract

The Department of Chemistry Malaysia has undergone a remarkable transformation, emerging as a dynamic multidisciplinary research institution committed to analytical excellence. Guided by a forward-thinking, “one step ahead” philosophy, the department consistently adapts to address national priorities, including forensic analysis, food safety, environmental protection, and public health. It also plays a critical role in responding swiftly and effectively during urgent outbreak situations.

At the heart of this transformation lies the Research and Instrumentation (R&I) Section under the Quality Management and Research Centre. Initially focusing on Capillary Electrophoresis (CE), High-Performance Liquid Chromatography (HPLC), Gas Chromatography (GC), and Mass Spectrometry (MS), the department advanced significantly under the Ninth Malaysia Plan (2006–2010). It embraced cutting-edge technologies like UPLC-MS/MS and GC-Large Volume Injection (LVI), resulting in the development of 48 innovative analytical methods for hazardous drugs, food safety, HALAL analysis, and water monitoring. By 2024, the department had further expanded its capabilities with Isotope Ratio Mass Spectrometry (IRMS), the Agilent LC-MS/MS system, and triple quadrupole GC-MS, achieving over 100 validated methods. These sophisticated techniques enable the department to respond rapidly to emerging challenges without compromising accuracy or adherence to international standards.

The department’s success is underpinned by a team of highly skilled professionals trained at leading local and international institutions, fostering a competitive edge in global analytical research. Strategic collaborations with universities and government agencies have strengthened proficiency testing, enhanced analytical methodologies, and elevated Malaysia’s capacity to address complex scientific challenges. Documented across 58 editions of its Chemistry Technical Bulletin and Annual Reports under MOSTI, the department’s achievements highlight a relentless commitment to innovation, public health, and global scientific excellence. This evolution underscores the Department of Chemistry Malaysia’s pivotal role in shaping a resilient and research-driven future.

Keywords: Evolution of Multidisciplinary Research, Advanced Instrumentation, Method Development & Collaboration, Outbreak Management, Scientific Publications

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A PRELIMINARY STUDY OF THE LOCAL RICE BREEDS USING ISOTOPE RATIO MASS SPECTROMETRY

Mohamad Izharudin Che Amat, Siti Sarah Abdul Aziz, Umami Hafiza Abdul Razak, Syaiphol Izani Che Man, Mohd Roushan Fiqir

Department of Chemistry Malaysia, Petaling Jaya, Selangor, Malaysia

Corresponding author: izharudin@kimia.gov.my

Abstract

The objective of this study was to develop a technique for determining the geographic origin of local rice in Malaysian market. The rice samples included products grown in Malaysia. A total of eleven different rice breeds were obtained from Malaysian Agricultural Research and Development Institute (MARDI). In peninsular Malaysia, Paddy is intensively planted in the west coast (Perlis, Kedah, Perak, and Selangor) and east coast areas (Kelantan, Terengganu and Pahang). We analyzed various sea turtle samples using Isotope Ratio Mass Spectrometry (IRMS), focusing on the stable isotope ratios of carbon ($\delta^{13}\text{C}$) and nitrogen ($\delta^{15}\text{N}$). Statistical methods, including boxplots, outlier tests, principal components analysis (PCA), and discriminant analysis (DA), were employed to analyze the data. By combining four chemometric techniques based on different principles and determination criteria, the geographic origin of rice was determined. The predictions made by cross-validation were around 90% accurate. The result demonstrated that IRMS stable isotope ratios combined with several chemometric techniques could be an effective tool for determining the geographic origin of locally grown rice.

Keywords: IRMS, rice, chemometric data analysis, stable isotope analysis

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BEYOND STANDARDS: THE ADVANCEMENTS IN CALIBRATION AT THE DEPARTMENT OF CHEMISTRY MALAYSIA

Irain Bahari, Norliza Abd Hamid, Yusnita Osman

Calibration Section, Department of Chemistry Malaysia,

Petaling Jaya, Selangor, Malaysia

Corresponding author: irain@kimia.gov.my

Abstract

The Calibration Section at the Department of Chemistry Malaysia plays a pivotal role in ensuring the accuracy, precision, and reliability of laboratory measurements. Accredited by Standards Malaysia (SAMM 061) in accordance with ISO/IEC 17025:2017 requirements, the section has continually expanded its calibration services since its inception in 2004. Initially focusing on mass and temperature-controlled enclosures—including freezers, ovens, incubators, chillers, water baths, and furnaces—the scope was broadened in 2023 to include liquid-in-glass thermometers and micropipettes. This expansion has enabled the issuance of over 300 calibration certificates annually.

To meet the increasing demands for high-performance chemical analysis, the department has embraced innovative calibration methodologies. These include the implementation of automated calibration systems, and the development of in-house procedures tailored for specialized equipment. The integration of digital platforms has further enhanced traceability and consistency, reinforcing the department's commitment to upholding both national and international calibration standards.

Continuous advancements in calibration are essential to support scientific research, industrial applications, and regulatory compliance. By driving innovation in metrology, the Department of Chemistry Malaysia significantly contributes to the global pursuit of standardization and excellence in laboratory measurements. These efforts not only enhance analytical accuracy but also position the department as a leader in global measurement harmonization.

Keywords: calibration, metrology, mass, heat enclosure, analytical accuracy, measurement harmonization, advanced calibration

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MODIFICATION OF BDD SURFACE BY ELECTROCHEMICAL REDUCTION OF DIAZONIUM SALTS FOR BIOSENSOR APPLICATIONS

Peter Čambal^{a,*}, Karmelita Hubčuková^a, Karolina Schwarzová-Pecková^a

^aDepartment of Analytical Chemistry, Faculty of Science, Charles University, Prague, Czech Republic

*Corresponding author: cambalp@natur.cuni.cz

Abstract

Boron doped diamond (BDD) is an electrode material well renowned for its high versatility, exceptional electrochemical properties, chemical stability and biocompatibility^{1,2}. These characteristics make BDD an ideal candidate for applications in electrochemistry, *e.g.* sensing or degradation of organic compounds. However, modification of the BDD surface is often required to create a rational design and enhance its properties for biosensor applications³.

Electrografting, as a quick and robust method for covalent modification, enables attachment of organic moieties, bearing various functional groups⁴. Generally, electrografting can be performed in an oxidative (*e.g.* oxidation of primary aromatic amines) or a reductive (*e.g.* electrochemical reduction of diazonium salts) way. Cyclic voltammetry and electrochemical impedance spectroscopy combined with spectral methods, such as X-ray photoelectron spectroscopy, are often used to confirm the presence of grafted layers and functional groups.

Introducing nitro and azo functional groups onto the BDD surface is of particular interest, because they may open pathways to further functionalization of the surface by reduction to amino group, which is beneficial for attachment of biomolecules, such as enzymes.

In this study, reductive electrografting of organic molecules introducing nitro and azo functional groups onto the BDD surface was investigated. The procedure consisted of electrochemical reduction of diazonium salts (4-nitrobenzene diazonium and GBC sulfate) utilizing cyclic voltammetry. The presence of organic layers after grafting was confirmed by cyclic voltammetry measurements with inner ($[\text{Fe}(\text{CN})_6]^{3-/4-}$) and outer ($[\text{Ru}(\text{NH}_3)_6]^{3+/2+}$) sphere redox markers, as significant inhibition of heterogeneous electron transfer kinetics is observed after grafting. Furthermore, the influence of BDD surface chemistry (H-terminated *vs.* O-terminated surface) on the electrografting procedure was investigated. Attempts to reduce the grafted nitro and azo groups by electrochemical and chemical (by reducing agents) ways will be discussed.

Acknowledgements: Financial support from Czech Science Foundation (project GAČR 23-05688S) and Grant Agency of Charles University (project 80124) is gratefully acknowledged.

Keywords: boron doped diamond, grafting, surface functionalization, electrochemical reduction, diazonium salts

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DETERMINATION OF ORGANOCHLORINE PESTICIDE RESIDUES IN CHINESE HERBAL MEDICINES USING GAS CHROMATOGRAPHY - TANDEM MASS SPECTROMETRY (GC-MS/MS): METHOD VALIDATION AND MEASUREMENT UNCERTAINTY ESTIMATION

Ella Lai-ming WONG^{a,*}, Jacky Ya-yin CHOI^a

^aAnalytical and Advisory Services Division, Government Laboratory of the Hong Kong Special Administrative Region

*Corresponding author: lmwong2@govtlab.gov.hk

Abstract

Chinese herbal medicines (Chms) are increasingly recognized worldwide for their significant nutritive and medicinal properties. The application of pesticides during the cultivation of Chms may be employed to manage pest populations and enhance both product yield and quality. However, if these pesticides are not utilized in accordance with established good agricultural practices, the resulting residues in Chms may pose potential risks to human health.

This study introduced a validated method that combined a modified QuEChERS (quick, easy, cheap, effective, rugged and safe) protocol with solid-phase extraction (SPE) preparation, coupled with gas chromatography – tandem mass spectrometry for the comprehensive monitoring of 26 organochlorine pesticides (OCPs) in Chms. A wide array of Chm matrixes, including 8 representative medicinal parts, was selected in the study to ensure the method is applicable to most Chinese raw herbs in the local market.

Various combinations of commercially available dispersive solid-phase extraction (dSPE) and SPE were utilized for effective clean-up of the complicated matrixes in the Chinese raw herbs. In order to mitigate the strong matrix effects, the matrix-matched calibration with isotopically labelled standards was employed which exhibited a linear range up to 350 µg/L and correlation coefficient $R > 0.995$; and whereas the difference between the actual and calculated concentration was within 20% for all selected OCPs in the calibration. The analytical performance was rigorously validated through the analysis of OCPs spiked at three distinct concentration levels for each individual pesticide. Spike recoveries of the OCPs in the 8 representative medicinal parts typically ranged from 70 – 120%, with RSDs less than 20%. Measurement uncertainties of OCPs in the related matrixes were also evaluated.

The proposed method is simple, rapid, cost effective and applicable to a broad range of Chm matrixes, rendering more efficient monitoring of the 26 targeted OCPs in Chms from routine analysis.

Keywords: Organochlorine pesticides, Chinese herbal medicines, QuEChERS, Gas Chromatography – tandem mass spectrometry, Measurement Uncertainties

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GC-MS METHOD FOR ASSESSING THE DISTRIBUTION OF 2,4,6-TRINITROTOLUENE RESIDUES AFTER EXPLOSION

Daria Danilova^{a,*}, Viktoryia Varabyova^a

^aState Institution Scientific and Practical Center of the State Forensic Examination Committee of the Republic of Belarus

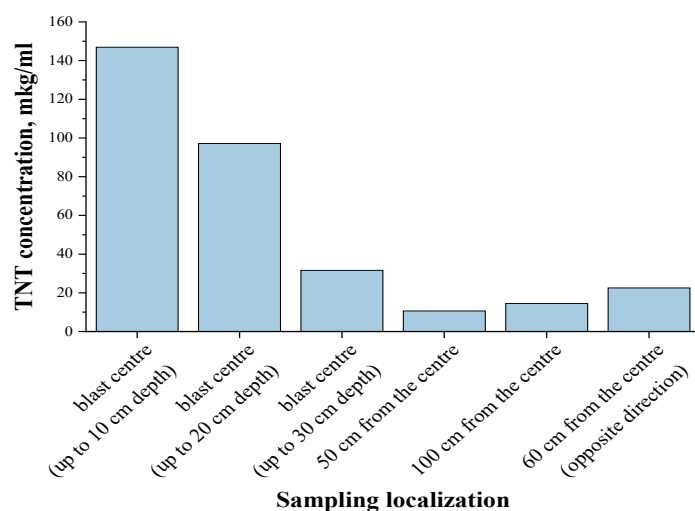
*Corresponding author: danilovad11@gmail.com

Abstract

The detection of explosive residues at an explosion site is one of the major challenges faced by forensic scientists. In this work, we used the gas chromatography-mass-spectrometry (GC-MS) method to investigate the content of 2,4,6-trinitrotoluene in soil samples collected from the blast site at different locations. The GC-MS method has been routinely used to detect nitro-organic explosives for over twenty years [1]. The aim of this work was to identify the soil areas with the highest analyte content to enable the subsequent development of techniques useful to forensic scientists who carry out sampling.

To achieve this goal, we collected soil samples from the center of the crater after the munitions explosion, from the surface and at different depths, as well as from the crater crests. The modified 8330B method was used to extract 2,4,6-trinitrotoluene from the soil [2]. Identification and quantitative determination of 2,4,6-trinitrotoluene in the samples were carried out on a TraceGOLD TG-SQC column (15 m × 0.25 mm × 0.25 μm), the helium flow rate was 1.2 ml/min, the oven temperature gradient was: 50 °C - hold for 3 min - heating at 15 °C/min to 280°C - hold for 10 min. The temperatures of the injector, transfer line and ion source were 280, 250 and 200°C, respectively. The range of recorded masses was from m/z 45 to 400. For the quantitative analysis of TNT m/z 210 ion monitoring was used.

Keywords: gas chromatography, mass-spectrometry, 2,4,6-trinitrotoluene, soil sampling



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THE SAMPLING LOCATION OF POLYMER-BONDED EXPLOSIVE TRACES

Viktoryia Varabyova^{a,*}, Daria Danilova^a

^aState Institution Scientific and Practical Center of the State Forensic Examination Committee of the Republic of Belarus.

*Corresponding author: viktoryia.vorobyova@gmail.com

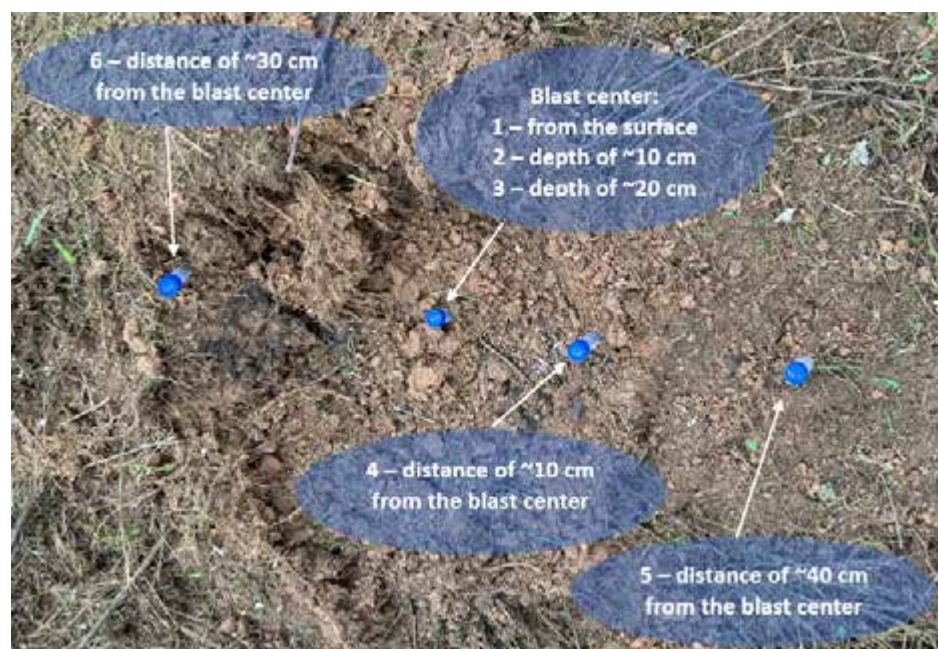
Abstract

The depth and localization of the sampling site play a crucial role in searching for explosive traces at the explosion site. Soil samples were collected after the explosion of the polymer-bonded explosive C-4 (an 1,3,5-trinitroperhydro-1,3,5-triazine (RDX)-based explosive) to identify the areas with the highest residue levels. Six samples of soil from the explosion site were collected in three parallel experiments, as shown in the figure below. The total number of samples was 19, including 1 blank sample.

Sample preparation was performed by liquid extraction. Methanol was used as a solvent. The extracts were analyzed by high-performance liquid chromatography with mass spectrometry and photodiode array detection (HPLC-MS/PDA). The quantity of RDX in soil samples after the explosion was estimated by an external standard method using a calibration curve. Identification of components was carried out by retention time and mass spectrum of reference RDX sample.

Based on the study results by HPLC-MS/PDA, the highest amount of RDX after the explosion is observed in the blast center at a depth up to 10 cm and the concentration of RDX decreases with increasing depth of sampling from the blast center.

Keywords: trace explosives, sampling location, RDX



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ARE ECSTASY STILL MDMA: THE CONTENTS OF ECSTASY TABLETS SEIZED IN PENANG STATE, MALAYSIA

Ng Choon Hiang^{a,*}, Suriati Shaiddin^a, Chang Kah Haw^b, Ahmad Fahmi Lim Abdullah^b

^aDepartment of Chemistry Malaysia, Pulau Pinang Branch, Malaysia.

^bSchool of Health Sciences, Universiti Sains Malaysia, Kelantan, Malaysia.

*Corresponding author: chng@kimia.gov.my

Abstract

The term “Ecstasy” was originally used to describe tablets containing 3,4-methylenedioxymethamphetamine (3,4-MDMA). According to the World Drug Report 2024 by the United Nations Office on Drug and Crime (UNODC), it was estimated that 20 million people had used ecstasy-type substances in 2022, representing 0.4% of the global population¹. However, the change in contents of ecstasy tablets have been reported in many countries in which they do not contain MDMA but other psychoactive substances mimicking its effects². To determine the composition and variation of ecstasy tablets submitted to the Narcotic Laboratory, Department of Chemistry Malaysia, Penang Branch. One hundred and thirty (130) ecstasy tablet samples were screened by portable Raman spectroscopy and characterized by gas chromatography-mass spectroscopy to identify the chemical compounds present inside the tablets. 107 out of 130 ecstasy tablets were found to contain MDMA, either existed alone (n=57; 43.8%) or with other controlled substances (n=50, 38.4%). Methamphetamine was found together with MDMA in a greater number of samples (n=27, 20.76%), followed by amphetamine (n=20, 15.38%), ketamine (n=13, 10%), and PMMA (n=3, 2.3%). 22 samples (16.92%) were detected with no MDMA but containing other controlled substances, poison or new psychoactive substances (NPS), and one sample (0.77%) was found with no active substance. This study also found that even ecstasy tablets with the same logo and physical appearance varied in their composition of active ingredients. There was variability in the chemical compositions of ecstasy tablets seized in the Penang State, Malaysia. Continuously sampling and monitoring of ecstasy composition is needed as routine forensic analyses of ecstasy tablets are restricted to the identification of the controlled substances.

Keywords: Ecstasy, 3,4-MDMA, GC-MS, portable Raman Spectroscopy, NPS

Graphic / Image



Variety of colour, shape, size, and imprints of ecstasy tablets encountered in this study.

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BEYOND THE HYPE: ESTABLISHING A UNIVERSAL FRAMEWORK FOR WEARABLE BIOCHEMICAL SENSOR STANDARDS

**Paolo Bollella,^{1,2} Derek Craston, Ruchi Gupta,³ Zoltán Mester,⁴ Tsuyoshi Minami,⁵ Takae Takeuchi,⁶
Joseph Wang,⁷ Luisa Torsi^{1,2,*}**

¹ *Department of Chemistry, University of Bari Aldo Moro, Via E. Orabona, 4 – 70125 Bari (Italy).*

² *CSGI@UniBa, University of Bari Aldo Moro, Via E. Orabona, 4 – 70125 Bari (Italy).*

³ *School of Chemistry, University of Birmingham, Birmingham, B15 2TT, UK.*

⁴ *Metrology Research Center, National Research Council Canada, Ottawa, Ontario, K1A0R6, Canada*

⁵ *Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan.*

⁶ *Division of Materials and Manufacturing Science, Graduate School of Engineering, The University of Osaka,
Suita, Osaka, 565-0871, Japan*

⁷ *Department of Chemical and Nano Engineering, University of California San Diego, La Jolla, CA, 92093, USA*

**Corresponding author: paolo.bollella@uniba.it*

Abstract

The field of wearable biochemical and chemical sensors has rapidly evolved, enabling non-invasive and continuous health monitoring through sweat, saliva, interstitial fluid, and other biofluids. However, the absence of standardized terminology, performance benchmarks, and regulatory guidelines has led to inconsistencies in device classification, data interpretation, and clinical validation. [1-3] Current definitions of wearable biosensors, chemical sensors, and bioelectronic devices often overlap, creating ambiguities in the literature. Additionally, key performance metrics, such as sensitivity, specificity, response time, and stability, are inconsistently reported, hindering cross-comparison of sensor performance. A lack of universally accepted biofluid-analyte correlation models further complicates the clinical translation of these technologies. [3] To address these gaps, this study highlights the need for harmonized terminology, standardized performance metrics, and regulatory frameworks to facilitate scientific progress and commercial adoption. Establishing clear benchmarking standards, data interpretation protocols, and clinical validation pathways will improve the reproducibility, reliability, and clinical impact of wearable biochemical sensors. A systematic effort to define these aspects will accelerate the integration of wearable biosensors into healthcare, diagnostics, and digital health applications. [4]

This work is supported by IUPAC with the project 2023-006-1-500 “Assessing the need for terminology, standards and guidelines for wearable devices that provide chemical/biochemical measurement readouts”.

Keywords: wearable biochemical sensors, standardized terminology, biofluids, healthcare and diagnostics, digital health.

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AN AMPEROMETRIC GLUCOSE BIOSENSOR BASED ON NANOZYME AND GLUCOSE OXIDASE MODIFIED ELECTRODE

Asta Kausaite-Minkstimiene^{a,*}, Austėja Orintaite^a, Aiste Krikstaponyte^a, Almira Ramanaviciene^a

^aNanoTechnas – Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko st. 24, LT-03225 Vilnius, Lithuania

*Corresponding author: asta.kausaitė@chf.vu.lt

Abstract

Although the first glucose biosensor was described by Clark and Lyons as early as 1962,¹ the development of glucose biosensors remains relevant to this day. And this is not surprising, because more than 800 million people around the world have diabetes,² and glucose biosensors are a very important analytical tool for both diagnosing diabetes and monitoring blood glucose fluctuations. This monitoring allows you to make informed decisions about medication dosages, dietary choices, and lifestyle changes, thereby reducing the risk of diabetes-related complications.³ Due to simple operation principle, amperometric glucose biosensors, whose operation is usually based on the oxidation of glucose by molecular oxygen catalyzed by immobilized glucose oxidase, are the most commonly developed glucose biosensors.⁴ However, despite high sensitivity and selectivity for glucose, short response time, and the possibility of being miniaturized and portable, these biosensors also have drawbacks, such as interference from other electroactive compounds or limited long-term stability, which make glucose determination inaccurate.⁵ New possibilities are opened up by nanozymes - synthetic materials that mimic the catalytic functions of natural enzymes.⁶ Various types of nanozymes are used in the field of biosensor development, depending on their material composition, including metal nanoparticles, metal oxides, carbon nanotubes and graphene. However, due to their reliable and stable catalytic properties, metallic nanoparticles composed of one or more metals are probably the most commonly used.⁷ Nanozymes of this type often exhibit strong enzyme-like activity because they can easily donate or accept electrons during redox reactions. Therefore, the integration of nanozymes into amperometric biosensors allows for significant improvements in their performance. As a consequence, this work presents the development and investigation of an amperometric biosensor based on a nanozyme and glucose oxidase modified graphite rod electrode for rapid, selective, and sensitive detection of glucose.

Keywords: glucose biosensor, glucose oxidase, nanozyme.

Acknowledgment

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FORENSIC CHALLENGES IN PATERNITY TESTING: A CASE OF MOLAR PREGNANCY

**Mohammad Azhar bin Mat Zin^{a*}, Muhamad Sufiyan bin Azah^a
Mohd Shafizi bin Ab Aziz^a**

^a*Forensic DNA Section of Eastern Zone, Department of Chemistry Malaysia Terengganu State*
Corresponding author: mohammadazhar@kimia.gov.my

Abstract

DNA paternity testing is a widely used forensic method to determine biological relationships with high accuracy. Standard samples include blood, buccal swabs, hair, and other bodily fluids. However, forensic cases involving product of conception (POC) samples can be challenging due to the difficulty in distinguishing foetal from placental DNA at the screening stage as well as interpreting the final DNA profile. This case study presents a forensic paternity investigation where a POC sample yielded a DNA mixture of two female profiles with various mixture ratio between the two contributors across all replicates. As expected, the mother's genotype was consistently present across all replicates. However, a second female contributor ("Female 1") was also detected, exhibiting only homozygous alleles across all loci, with a genotype largely inconsistent with the mother's genotype. Notably, the alleles of "Female 1" closely matched the alleged father's genotype, raising initial concerns of contamination or handling errors during sampling. Further literature review revealed that the genetic profile of "Female 1" was consistent with a complete molar pregnancy—a rare condition involving an abnormal fertilization event leading to a non-viable, genetically unique conceptus. The findings underscore the importance of analyst expertise in distinguishing biological phenomena from potential contamination in forensic DNA interpretation. This case highlights the need for awareness of molar pregnancy in forensic investigations involving POC samples, as misinterpretation could lead to incorrect conclusions in paternity cases.

Keyword: Paternity testing, product of conception, molar pregnancy

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HIGHLY SENSITIVE ELECTROCHEMICAL IMMUNO-SENSORS USING ENZYMATIC PRECIPITATION OF PRUSSIAN BLUE

Sathyan Babu^a, Eunji Tak^a, Haesik Yang^{a*}

^aDepartment of Chemistry, Pusan National University, Busan 46241, Korea.

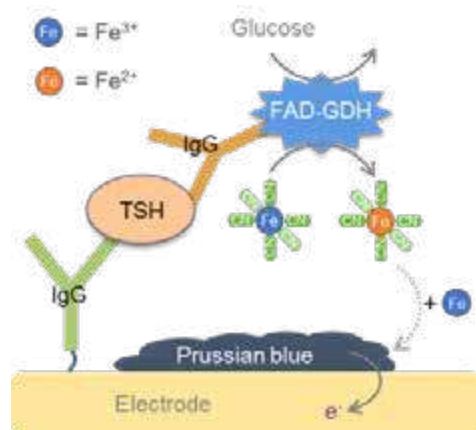
*Corresponding author: hyang@pusan.ac.kr

Abstract

Sensitive and/or multiplex electrochemical biosensors often require efficient (bio)catalytic conversion of substrates into insoluble electroactive products. The enzymatic formation and precipitation of coordination polymers under mild conditions offers a promising solution for this purpose. Herein, we report the enzymatic precipitation of Prussian blue (PB), a highly electroactive and ion-transporting coordination polymer, on an immunosensing electrode for application in a sensitive electrochemical immunosensor for detecting thyroid-stimulating hormone (TSH). Five pairs of redox enzymes and their specific reductants were examined to achieve rapid PB precipitation and electrochemical oxidation. Among these pairs, -insensitive flavin adenine dinucleotide-dependent glucose dehydrogenase (FAD-GDH) paired with glucose yielded the highest electrochemical signal-to-background (S/B) ratio. FAD-GDH catalyzed the conversion of to , which coordinated with , leading to PB formation and subsequent precipitation through repeated conversions. The resulting PB precipitate, with its close proximity to the electrode, facilitated rapid electrochemical oxidation and generated a strong electrochemical signal. Notably, the precipitation and electrochemical oxidation of PB were more effective than those of its analogues. When applied to a sandwich-type immunosensor for TSH detection, the enzymatic PB precipitation achieved a calculated detection limit of approximately 2 pg/mL in artificial serum, covering the clinically relevant range. These findings indicate the potential widespread utility of PB precipitation and electrochemical oxidation for sensitive multiplex biomarker detection.

Keywords: Prussian Blue, Enzymatic Precipitation, Electrochemical Immunosensor, Thyroid-Stimulating Hormone, Glucose Dehydrogenase

Graphic / Image



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SENSITIVE XANTHINE DETECTION USING XANTHINE DEHYDROGENASE AND $[\text{Os}(\text{bpy})_2\text{Cl}_2]^+$ WITH LOW INTERFERENCE

Taeyeon Yoo^a, Seonhwa Park^a, Haesik Yang^{a*}

^aDepartment of Chemistry,

Pusan National University, Busan, 46241, Korea.

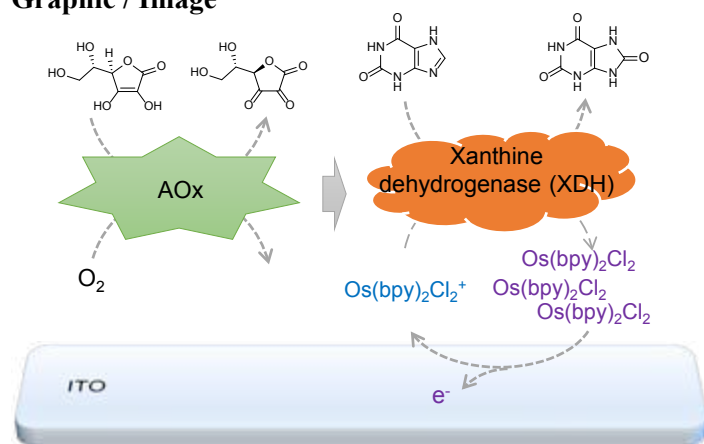
*Corresponding author: hyang@pusan.ac.kr

Abstract

Enzyme-based biosensors utilizing mediated electrochemical detection offer a simple, efficient, and cost-effective approach for xanthine detection. However, the presence of electro-active interfering species such as ascorbic acid (AA) poses significant challenges in achieving both sensitivity and selectivity, particularly in biological fluids. The direct and mediated oxidation of AA increases electrochemical background levels, complicating the accurate detection of xanthine. To address this issue, ascorbate oxidase (AOx) is introduced to convert AA into an electro-inactive product. However, if AA is not completely removed, residual AA contributes to elevated background signals, reducing the reliability of the measurement. Additionally, excessive AOx may slowly oxidize the reduced form of the electron mediator, leading to decreased signal intensity. To minimize these interferences, a two-step incubation process is implemented, along with optimization of AOx concentration. In this approach, AA is first fully oxidized by AOx before an electron mediator is introduced into the system. Furthermore, to enhance the electrochemical signal-to-background ratio, various combinations of xanthine-oxidizing enzymes and electron mediators are systematically evaluated. Among the tested conditions, the pairing of xanthine dehydrogenase (XDH) with $[\text{Os}(\text{bpy})_2\text{Cl}_2]^+$ exhibits the most favorable performance, providing a high signal while maintaining low background levels. Under these optimized conditions, xanthine detection in artificial serum achieves a detection limit of approximately 500 nM. These findings demonstrate the potential applicability of this approach in clinical diagnostics and biochemical research, where reliable and sensitive xanthine detection is essential.¹

Keywords: ascorbate oxidase, ascorbic acid, electrochemical detection, xanthine dehydrogenase, xanthine detection

Graphic / Image



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GOLD NANOPARTICLE-MEDIATED ELECTRON TRANSFER FROM AMMONIA-BORANE TO $\text{Ru}(\text{NH}_3)_6^{3+}$ FOR HIGHLY- SENSITIVE BIOSENSING

Seonhwa Park^a, Seongjin Park^a, Haesik Yang^{a*}

^aDepartment of Chemistry,

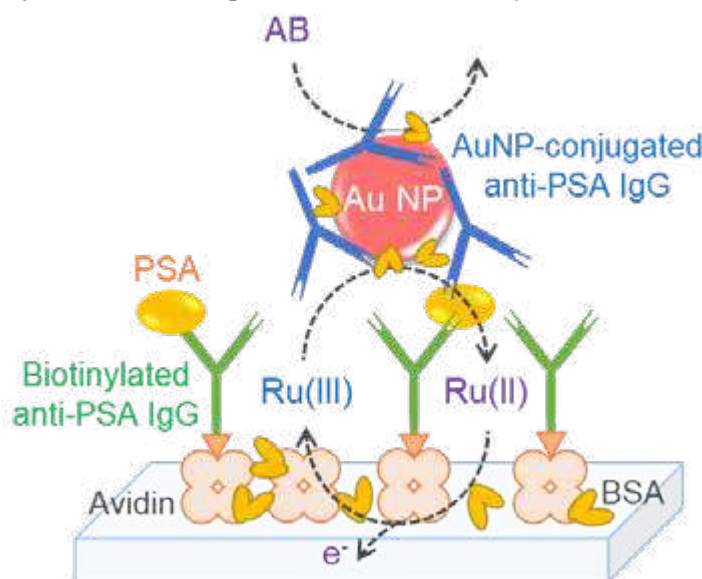
Pusan National University, Busan, 46241, Korea

*Corresponding author: hyang@pusan.ac.kr

Abstract

Metal nanoparticle (NP)-catalyzed electron transfer (ET) from a reducing agent to a metal complex is essential for signal amplification in biosensors. Efficient ET requires the metal complex to undergo fast outer-sphere reactions, exhibit high water solubility, and effectively penetrate bio/organic layers on metal NPs. In this study, we identify $\text{Ru}(\text{NH}_3)_6^{3+}$ as an optimal candidate for this process. Among various reducing agents, ammonia-borane (AB) facilitates rapid metal NP-catalyzed ET, with Au, Pt, and Pd NPs demonstrating comparable catalytic activities. The pseudo second-order rate constant for 20-nm Au NP-catalyzed ET from AB to $\text{Ru}(\text{NH}_3)_6^{3+}$ ($1.4 \times 10^8 \text{ M}^{-1}\text{s}^{-1}$) approaches the diffusion-controlled rate constant. Notably, even in the presence of passively adsorbed immunoglobulin G and bovine serum albumin on Au NPs, catalytic activity remains largely unaffected. When applied to prostate-specific antigen detection in human serum, Au NP-catalyzed ET enables a low detection limit of 10 pg/mL. These results underscore the potential of $\text{Ru}(\text{NH}_3)_6^{3+}$ and AB in the development of biosensors based on rapid catalytic reactions.

Keywords: Au nanoparticle, biosensor, catalytic label, electrochemical detection, $\text{Ru}(\text{NH}_3)_6^{3+}$



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DEVELOPMENT AND OPTIMIZATION OF AN ANALYTICAL METHOD FOR AIR POLLUTION MONITORING USING CANISTERS BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY WITH THERMAL DESORPTION (GC-MS-TD) TECHNIQUES

**Amran Ahmad, Mohd Rahmat Ramathani, Nur Hidayah Mohd Ran, Fatin Shahira Tasripin,
Wan Norfatihah Wan Omar Bakri, Nazarudin Ibrahim, Aziati Mokhtar**

Department of Chemistry Malaysia, Petaling Jaya, Selangor, Malaysia

**Corresponding author: amran@kimia.gov.my*

Abstract

This study aims to develop an analytical method for determining the levels of volatile organic compounds (VOCs) in air, adapted from the USEPA Compendium Method TO-15 using canisters. A total of 59 target compounds, ranging from propene to naphthalene, were collected by canisters and analyzed using Thermal Desorption (TD) coupled with Gas Chromatography-Mass Spectrometry (GC-MS). The analytical system used consists of a CIA Advantage-xr™ autosampler, Kori-xr™ water condenser, and UNITY-xr™ thermal desorber, all integrated into a GC-MS system. This setup efficiently collects and analyzes air samples by removing moisture and concentrating volatile compounds, enhancing measurement precision. Calibration was performed with concentrations ranging from 0.5 ppbv to 25 ppbv, ensuring adequate sensitivity to detect pollutants at very low levels. The analysis runtime was reduced from 41 minutes to 21 minutes, significantly accelerating the process and conserving time. To meet the performance criteria set for this method, two key factors were demonstrated: method detection limit (MDL) as low as 0.5 ppbv and audit accuracy within 30%. Both criteria were successfully achieved, fully complying with established guidelines for air quality monitoring.

Keywords: volatile organic compounds (VOCs), canister, USEPA TO-15, thermal desorption (TD), gas chromatography-mass spectrometry (GC-MS)

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FORENSIC CHARACTERIZATION OF METALLIC EVIDENCE: A COMPARATIVE STUDY OF XRF AND SEM-EDX TECHNIQUES

Syed Fariq Fathullah Syed Yaacob^a, Ahmad Zaeri Latahir^a, Chong Kah Wai^a,
Rusyidah Abdul Rahim^{a,*}

^aCriminalistic section, Forensic Science Analysis Center, Department of Chemistry Malaysia, Jalan Sultan, 46661 Petaling Jaya, Selangor Darul Ehsan, Malaysia.

*Corresponding author: rusyidah@kimia.gov.my

Abstract

Accurate elemental analysis is critical in forensic investigations, especially in cases involving metallic evidence such as firearms and ballistics ¹, forgery and trace evidence ², as well as theft and illicit trade ³ investigation. This study evaluates the detection capabilities of portable X-ray fluorescence (XRF) and scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) for forensic metallic evidence analysis. A comparative assessment was conducted on ten forensic-relevant metallic samples, including coins, bullets, jewellery, and standard gold. Elemental detection rates were statistically analyzed using a paired t-test ⁴ and Bland-Altman ⁵ analysis to determine the agreement between the two methods. Results indicate that XRF detects a significantly higher number of elements per sample ($p < 0.05$), with an average detection count of 4.8 compared to 2.4 for SEM-EDX. The Bland-Altman analysis revealed a mean bias of -2.4, indicating that XRF consistently detects more elements, with limits of agreement ranging from -6.34 to 1.54. These findings highlight the complementary strengths of the two techniques, where XRF provides rapid, bulk elemental analysis in situ, while SEM-EDX offers high-resolution surface characterization in a controlled laboratory setting. The study underscores the necessity of an integrated approach to forensic material analysis, leveraging both techniques to ensure comprehensive elemental profiling of metallic evidence.

Keywords: XRF, SEM-EDX, forensic analysis, metallic evidence, elemental detection



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BORON-DOPED DIAMOND NANOMATERIAL FOR ELECTROANALYTICAL APPLICATION

Prastika Krisma Jiwanti

*Nanotechnology Engineering, Faculty of Advanced Technology and Multidiscipline, Universitas Airlangga,
Surabaya 60115, Indonesia*

Corresponding author: prastika.krisma@ftmm.unair.ac.id

Abstract

Boron-doped diamond (BDD) is well known for its outstanding electrochemical properties, including a wide potential window, low background current, and high chemical and physical stability¹. Due to these characteristics, BDD has been widely used as an electrode material in electrochemical analysis and electrocatalytic applications. In its nanoparticle form, known as boron-doped diamond nanoparticles (BDDNP), this material offers unique advantages, particularly in terms of easier modification and fabrication into composite materials, enhancing its versatility for specific applications. BDDNP can be utilized in the development of screen-printed electrodes for electrochemical detection. Various sensor applications, such as those for fluoroquinolones^{2,3}, azithromycin⁴, artificial sweeteners⁵, and bronchodilator drug⁶ will be explored. Fluoroquinolones, a class of quinolone antibiotics that includes ciprofloxacin (CIP), ofloxacin (OFL), and levofloxacin (LEV), are effective against gram-positive bacteria. Despite their therapeutic benefits, these antibiotics are frequently used in livestock as growth promoters, raising concerns about antibiotic resistance and residues in food products such as meat, milk, and eggs. This highlights the need for rapid and highly sensitive sensor devices. Here in, the discussion will be focus on the fabrication of functionalized BDDNP, various sensor validations, and analysis in real sample. The results of those experiments show that BDDNP could enhance the sensitivity of the sensor, has high stability, and could be produce as a cheap and portable sensor device (Fig.1).

Keywords: boron doped diamond nanomaterial, sensor, electrochemistry, fluoroquinolone,



Figure 1. Sensor device using screen printed diamond electrode

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ARE THESE METAL OBJECTS FROM SPACE? A CASE STUDY OF FORENSIC ANALYSIS OF METAL FRAGMENTS

Farah Ad-Din Nordin^{a,*}, Saiful Fazamil Mohd Ali^a, Mohd Izuan Othman^a

^a*Department of Chemistry Malaysia, Jalan Sultan, 46661 Petaling Jaya, Selangor Darul Ehsan*

^{*}*Corresponding author: farahaddin@kimia.gov.my*

Abstract

This study investigates the forensic examination of metal fragments recovered from unidentified objects that were received at the laboratory. This study employs non-destructive techniques which are the X-ray fluorescence (XRF) and Field Emission Scanning Electron Microscopy (FE-SEM) to analyze the elemental composition of the metal fragments. The goal is to assess whether the elemental composition of the fragments can be used to determine their origin; whether these fragments are from industrial, automotive, or aerospace applications or if they originated from space debris, such as satellite or rocket components. The results indicate a high presence of aluminum, magnesium, zinc and iron, suggesting possible applications in aerospace, automotive, or industrial sectors. This study highlights the effectiveness of forensic material analysis in identifying and classifying metal fragments from unidentified objects. The integration of XRF and FE-SEM analysis successfully determined the elemental composition of the samples, revealing potential origins in aerospace, automotive, and industrial sectors.

Keywords: elemental composition, non-destructive technique

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SMART CONNECTOR, INNOVATIVE SOLUTION TO TEMPERATURE CALIBRATION

Norliza Abd Hamid

Calibration Section, Department of Chemistry Malaysia,

Petaling Jaya, Selangor, Malaysia

Corresponding author: norliza@kimia.gov.my

Abstract

Temperature calibration is a fundamental aspect of thermophysical metrology within the Chemistry Department, ensuring the accuracy and reliability of temperature-controlled enclosures used in various scientific and industrial applications. Maintaining competitive Calibration Measurement Capabilities (CMC) among commercially accredited laboratories, the department produces approximately 400 calibration reports annually across its internal laboratories in Malaysia.

A key challenge in this process is the limited availability of temperature recorders, which are essential for accurate calibration. Conventional recorders are often expensive, scarce, and require extensive maintenance, posing logistical and financial constraints. To address these limitations, an innovative approach was adopted through the development and integration of a Smart Connector. This device mimics the multi-input functionality of traditional temperature recorders, allowing flexible and adaptable sensor-to-recorder connections without compromising measurement accuracy.

Calibration tests demonstrated that the Smart Connector exhibited no significant deviation in signal output when compared to standard commercial equipment, confirming its technical efficacy and reliability. Furthermore, the adoption of this solution resulted in an 80% reduction in operational costs, significantly improving efficiency and sustainability in calibration workflows. By offering a cost-effective, scalable, and technically robust alternative, the Smart Connector represents a major advancement in temperature calibration, with potential applications in diverse scientific and industrial settings.

Keywords: thermophysical metrology, smart connector, temperature calibration, temperature-controlled enclosures, calibration process, cost-effective innovation, sensor integration

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SCREENING SYNTHETIC CATHINONES MIXED WITH INSTANT COFFEE AND FRUIT JUICE POWDER USING HYDROPHOBIC CARBON DOT PROBES

Yao-Te Yen^{a*}, Huai-Han Chang^b, Yu-Ti Wang^a, Wei-Ting Chen^b, Yuh-Lin Liu^a, San-Chong Chyueh^a, and Chien-Fu Chen^b

^aDepartment of Forensic Science, Investigation Bureau, Ministry of Justice, Xindian Dist, New Taipei City 231209, Taiwan

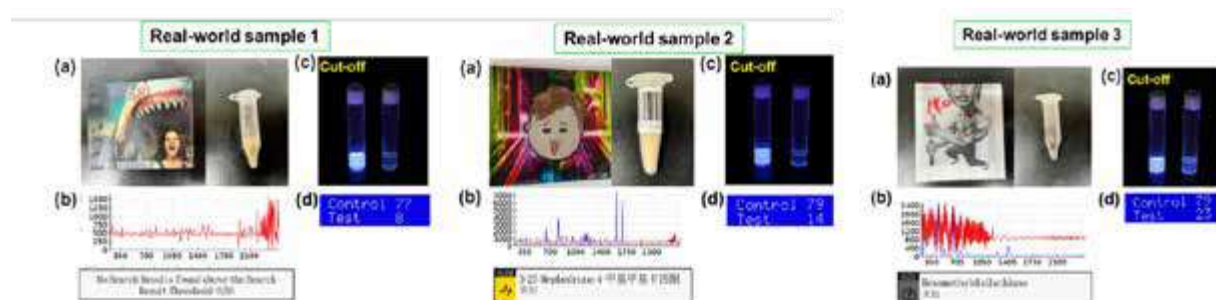
^bInstitute of Applied Mechanics, National Taiwan University, Taipei 10617, Taiwan

*Corresponding author: D05223113@ntu.edu.tw

Abstract

Synthetic cathinones, a category of new psychoactive substance (NPS) with diverse structures and appearances in forms such as powder, tablets, and pills, have caused severe social problems¹⁻². To make them attractive to teenagers, synthetic cathinones may be mixed with instant coffee and fruit juice powders. Difficulties in detecting these drugs in complex matrices complicate seizure of synthetic cathinones. Herein, a novel probe kit comprising hydrophobic tryptophan-carbon dots (htC-dots) with a liquid–liquid extraction procedure was used to detect 4-chloromethcathinone (4-CMC) and other synthetic cathinones mixed into instant coffee and fruit juice powder. Additionally, a self-made fluorescence detector controlled with an Arduino system was developed for the htC-dot probe kits. For 4-CMC, the dynamic ranges and detection limits were assessed as 0.125–0.75 mM and 0.08, respectively, for the microplate reader and as 0.625–5 mM and 0.42 mM, respectively for the self-made fluorescence detector. The sensory mechanism of the probe kit involved photoluminescence (PL) quenching of htC-dots through electron and hot electron transfer under an excitation wavelength of 302 nm. The matrix effects of five brands of instant coffee and fruit juice powder were evaluated, and a cut-off htC-dot solution was prepared to assess htC-dot probe kit accuracy. Finally, 24 real-world samples were tested using the htC-dot probe kits, and the results were confirmed using gas chromatography–mass spectrometry (GC–MS). The results suggested that the htC-dot probe kits have considerable potential for on-site screening of synthetic cathinones mixed into instant coffee and fruit juice powder.

Keywords: hydrophobic carbon dots, synthetic cathinones, fluorescence detectors, instant coffee and fruit juice powders



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CHEMICAL PROFILING OF NEW PSYCHOACTIVE SUBSTANCES (NPS) RECEIVED IN SARAWAK-A PILOT STUDY

^aAishah Abdul Aziz, ^aHazalinawati Zailani, ^bWan Nur Syuhaila Mat Desa &
^aBilling Anak Peter Raig

^a Narcotic Section, Forensic Science Analysis Division, Department of Chemistry Malaysia
Sarawak State

^b School of Health Sciences, University Science Malaysia (USM) Kubang Kerian, Kelantan
Corresponding author: wannurs@usm.my

Abstract

The rise of new psychoactive substances (NPS) presents a significant public health concern both nationally and globally. This study analysed seventeen NPS samples collected from three regions in Sarawak to determine their chemical composition and adulterants. Various analytical techniques were employed, including physical examination, screening color tests, thin-layer chromatography (TLC), attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR), gas chromatography-mass spectrometry (GC-MS)¹, and inductively coupled plasma mass spectrometry (ICP-MS)². Organic profiling revealed that Sunset Yellow was the primary dye used in the samples. Hence, the majority of NPS compounds belonged to the benzodiazepine (33%) and synthetic cathinone (27%) groups, with mannitol and caffeine identified as the predominant adulterants³. Furthermore, trace elements such as calcium and mercury were detected. Notably, samples retrieved from Kuching (K9) and Bintulu (BT1) exhibited similar chemical characteristics. These findings highlight the diverse composition of NPS samples and provide valuable forensic and intelligence insights for narcotics enforcement agencies in Sarawak and Malaysia.

Keywords: NPS, TLC, GC-MS, ATR-FTIR, ICP-MS.

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DEVELOPMENT OF SURFACE PLASMON INTERFACE EXCITATION ION SOURCE

Yongyi Li^a, Qian An^a, Zhihui Huang^a, Xiangyu Wang^a, Wenxin Wang^a, Zhenwei Wei^{a,*}

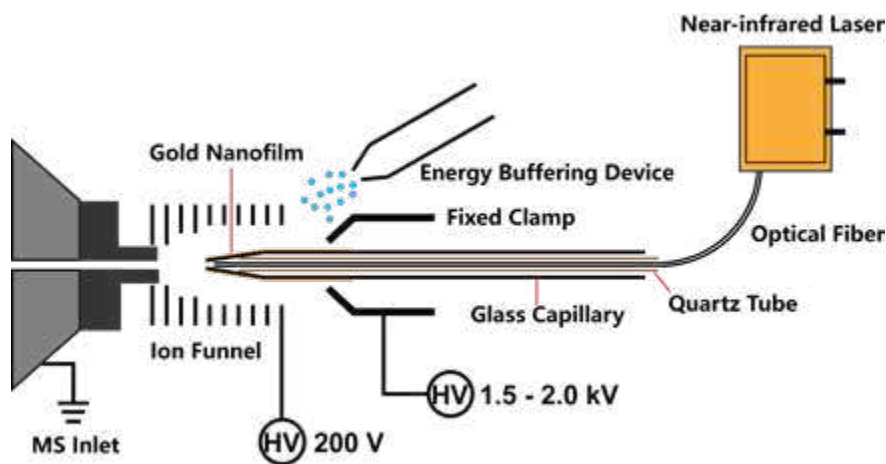
^aCollege of chemistry and molecular sciences, Wuhan University, Wuhan 430072, China

*Corresponding author: weizw2021@whu.edu.cn

Abstract

A new ambient surface plasmon interface excitation ionization method is developed and applied to the ionization of small molecules with broad polarity ranges, as well as macromolecules such as peptides, proteins, and nucleic acids. This technique achieves molecular excitation and ionization through surface plasmon resonance effects on metallic thin films. After laser excitation, electronic oscillations at the metal-medium interface are induced, and the energy from these oscillations is converted into thermal and chemical energy for the vaporization and ionization of neutral analytes.¹ This matrix-free laser desorption ionization technique employs nanoscale metallic films as energy conversion media, while adopting rear-illuminated laser excitation to avoid direct laser-sample interaction, thereby enabling soft ionization. In this work, the metal-dielectric interface was constructed on the tapered region of glass capillaries. The laser was focused when passing through the tapered region and induced surface plasmon.² Direct solution dipping³ allows rapid analysis of compounds spanning wide polarity ranges, including aromatic compounds, saccharides, cholesterol, lipids, small-molecule drugs, as well as large biomolecules such as peptides, proteins, and nucleic acids. Using this platform, we achieved in situ sampling and direct analysis of single cells. Furthermore, selective excitation of analytes was accomplished through laser modulation for precise surface energy control.

Keywords: mass spectrometry, ambient laser desorption ionization, surface plasmon, interfacial energy control, single cell analysis.



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A COMPARATIVE STUDY OF OPEN AND CLOSED VESSEL ACID DIGESTION FOR HEAVY METAL ANALYSIS USING INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY (ICP-MS)

Madiah Ahmad*, Sitti Mariam Nunurung, Kalaimangai Sugumaran, Haliza Hasan, Nazarudin Mohamed@Ibrahim

Department of Chemistry Malaysia, Petaling Jaya, Selangor, Malaysia.

**Corresponding author: madiah@kimia.gov.my*

Abstract

This study compares two acid digestion methods, namely open vessel (hot plate) and closed vessel (microwave digester), which were used to prepare dry-fallout samples for determining the elemental composition. The analysis of nine heavy metal elements, including calcium (Ca), copper (Cu), iron (Fe), lead (Pb), magnesium (Mg), manganese (Mn), mercury (Hg), nickel (Ni), and zinc (Zn), was conducted using Inductively Coupled Plasma-Mass Spectrometry (ICP-MS). The analyte recovery rates and coefficients of variation (CV) obtained from both digestion methods were found to be nearly identical. However, the microwave digester demonstrated slightly superior recovery, particularly for volatile elements like mercury. While both methods provided comparable results in terms of analyte recovery, the microwave digestion method offered enhanced safety due to its closed vessel system and enabled a more controlled digestion process, leading to reliable and consistent results. These advantages make the microwave digester the preferred choice for sample preparation, especially in environments where safety and the recovery of volatile elements are crucial.

Keywords: acid digestion, open vessels, close vessels, sample preparations, ICP-MS (Inductively Coupled Plasma-Mass Spectrometry)

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DEVELOPMENT AND EVALUATION OF PORTABLE NIR TECHNOLOGY FOR THE IDENTIFICATION OF CANNABINOIDS IN PLANT MATERIALS

Hazirah Hasim*, Rosman Bawok, Nor Vickneswary, Dr Vanitha Kunalan

Forensics Science Analysis Center, Department of Chemistry Malaysia, Petaling Jaya, Selangor.

**Corresponding author: hazirah@kimia.gov.my*

Abstract

Cannabis, scientifically known as *cannabis sativa*, means any part of any plant of the genus cannabis from there is found to be present resin irrespective of its quantity, and by whatever name the plant may be designated. ‘Street’ names for Cannabis: marijuana, dope, pot, grass, weed, head, mary jane, doobie, bud, ganja, hashish, hash and bhang. Cannabinoids (kuh-NA-bih-noyd) is a type of chemical in marijuana that causes drug-like effects all through the body, including the central nervous system and the immune system. At present, it is illegal to grow any type of cannabis in Malaysia. Consumption of cannabis, whether in raw or processed form, is a punishable offence under the Dangerous Drugs Act 1952 (DDA). The need for rapid and non-destructive analytical techniques is crucial today, especially for forensic work in the field and in the laboratory. The development and production of portable equipment has greatly assisted and facilitated analyst in carrying out task in Department of Chemistry Malaysia. Cannabis is a frequently received seized material sample in the laboratory for confirmation purposes. Typically, the analysis scheme for cannabis confirmation involves several examinations and tests before it is confirmed as a “cannabis”. These tests include identifying the plant material as belonging to the cannabis genus and identifying cannabinoids. Handheld microNIR is used to identify cannabinoids and compared with thin layer chromatography (TLC) techniques using the same cannabis samples. The presence of major cannabinoids in cannabis, namely Tetrahydrocannabinol (THC), Cannabinol (CBN) and Cannabidiol (CBD) are compared between the two techniques. Unlike TLC, which requires intensive sample preparation, the use of numerous chemicals and solvents, and ultimately produces chemical waste. The NIR spectrometer provides real-time, on-site analysis with minimal environmental impact, in line with green technology and sustainable practices.

Keywords: Cannabis, *cannabis sativa*, cannabinoids, near infrared (NIR), forensic science

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LASER-ABLATED NICKEL NANOPARTICLES AS AN ELECTROCHEMICAL PLATFORM FOR INSULIN DETECTION

Renáta Oriňaková^{a,b*}, Ivana Šišoláková^a, Martin Cvek^b

^aDepartment of Physical Chemistry, Faculty of Science, Pavol Jozef Šafárik University in Košice, Moyzesová 11, 040 01, Košice, Slovak Republic

^bCentre of Polymer Systems, Tomáš Baťa University in Zlín, Třída Tomáše Bati 5678, 760 01, Zlín, Czech Republic

*Corresponding author: renata.orinakova@upjs.sk

Abstract

The precise and sensitive determination of insulin is crucial for diabetes management and biomedical applications. In this study, we explore laser-ablated nickel nanoparticles (NiNPs) as an effective electrochemical sensor modification for insulin determination [1]. The NiNPs were synthesized via a laser ablation technique, ensuring high purity and controlled particle size distribution [2]. The NiNPs modified electrode showed enhanced electrocatalytic activity toward insulin oxidation compared to electrode without nanoparticles, resulting in improved sensitivity and selectivity. Electrochemical characterization, including cyclic voltammetry confirmed the superior performance of the NiNP-modified electrode compared to unmodified sensors. The developed sensor demonstrated a low detection limit (0.28 μM), a broad linear range (0.25 μM –5 μM) with correlation coefficient $R^2=0.99$, and excellent reproducibility. Furthermore, interference studies showed minimal effects from common physiological species, highlighting the practical applicability of the developed sensor. The laser ablation method provides a green and efficient route for nanoparticle synthesis, making it a promising approach for advanced electrochemical biosensors.

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Keywords: nickel nanoparticles, laser ablation, insulin, electrochemical sensor, diabetes

Graphic / Image

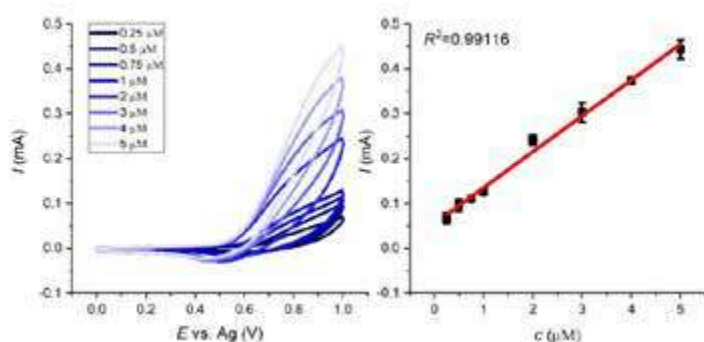


Figure 1: Cyclic voltammograms of various insulin concentrations (0.25 μM – 5 μM) in PBS and 0.1 M NaOH at scan rate of 0.1 V s^{-1} in a potential range -0.5 V to +1 V (A). The dependence of peak current on the insulin concentration fitted by a linear function (B).

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OPTIMIZING AUTOMATED DNA EXTRACTION AND PURIFICATION FOR FORENSIC SAMPLES USING THE EZ1&2™ DNA INVESTIGATOR® KIT ON THE EZ2® CONNECT FX WITH THE CASEWORK TRACE PROTOCOL

Dayang Zarifah Ataillah Awang Aemeran^{a*}, Normazlina Zainudin^a,
Nur Fadzlina Yahaya^a, Faten Najah Mohd Kassim^a, Mahzan Md Tab^a,
Siti Hajar Hussin^a and Nor Aidora Saedon^a

^a Department of Chemistry Malaysia, Petaling Jaya

*Corresponding author: zarifah@kimia.gov.my

Abstract

Forensic DNA analysis plays a crucial role in solving criminal cases, identifying individuals, and establishing biological relationships. One of the primary challenges in forensic casework is extracting and purifying DNA from challenging and low-template samples, such as trace evidence and degraded biological materials. The efficiency of DNA extraction directly impacts the success of downstream applications including short tandem repeat (STR) analysis. The EZ1&2™ DNA Investigator® Kit, integrated with the EZ2® Connect Fx system, provides an automated, efficient, and contamination-minimized solution for forensic DNA extraction. This platform utilizes magnetic-bead technology to ensure high-quality DNA yields, free from inhibitors and contaminants, making it suitable for forensic applications. The Casework Trace Protocol is specifically designed to maximize DNA recovery from low-level, degraded, or trace forensic samples, optimizing extraction efficiency while maintaining high reproducibility and reliability. This study aims to evaluate the performance and efficiency of the Casework Trace Protocol on the EZ2® Connect Fx system. Mock forensic samples were prepared from a single identified female source, consisting of six serial blood dilutions ranging from 0.005 µl to 1 µl. Each sample from the dilution series was analyzed in quadruplicate using the Casework Trace protocol. The automated DNA extraction focused on assessing the system's sensitivity, selectivity, repeatability, and reproducibility. The results demonstrated consistent and reliable DNA yields across varying sample dilutions. Therefore, this study highlights the effectiveness, efficiency, and reliability of the EZ1&2™ DNA Investigator® Kit for extracting DNA from challenging forensic samples, reinforcing its value in forensic and human identification laboratory.

Keywords: magnetic-bead technology, EZ1&2™ DNA Investigator® Kit, EZ2® Connect Fx, casework trace protocol, short tandem repeat (STR) analysis

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METHOD VALIDATION FOR THE DETERMINATION OF INORGANIC ARSENIC IN SEAWEED USING HPLC-ICP-MS

Ying Ying Low^{a,*}, Hairul Nizwan Bin Ab Manap^a

^a Department of Chemistry Malaysia

*Corresponding author: lowyy@kimia.gov.my

Abstract

Seaweed contains both inorganic and organic arsenic, with inorganic arsenic being more toxic and carcinogenic. Human exposure to arsenic can occur through seaweed consumption, making it essential to conduct arsenic speciation studies for accurate toxicity assessment. A selective and sensitive analytical method was validated for quantifying inorganic arsenic species, specifically arsenate (AsV) and arsenite (AsIII), in seaweed using high-performance liquid chromatography coupled with inductively coupled plasma mass spectrometry (HPLC-ICP-MS). Seaweed samples were extracted using 0.2% (v/v) nitric acid and heated at 95 °C. The extracts were then analyzed for arsenic species concentrations using HPLC-ICP-MS with a C18 MG column and a mobile phase containing octane sulfonic acid as an ion-pair reagent. The method exhibited good linearity within the range of 0.4 µg/L to 10 µg/L and is applicable for quantifying inorganic arsenic in seaweed samples at concentrations ranging from 0.1 mg/kg to 2.5 mg/kg. The limit of detection (LOD) was determined to be 0.03 mg/kg, while the limit of quantitation (LOQ) was 0.1 mg/kg. The average recoveries for fortified samples ranged from 80% to 110%, with precision below 12%. This straightforward method demonstrated the necessary detection limits and performance characteristics, meeting regulatory and standard requirements.

Keywords: inorganic arsenic, HPLC-ICP-MS

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HANDHELD FTIR UNMASKS SIMETHICONE AND POLYDIMETHYLSILOXANE IN ILLEGAL BREAST FILLERS

Siti Fairuz Rosli^{a,*}, Zul Helmi Salleh^a, Mohamad Shazrul Izzuan Azami^a, Sharmilah Kuppusami^a,
^aToxicology Division, Department of Chemistry Malaysia, Jalan Sultan, 46661 Petaling Jaya, Selangor, Malaysia.

**Corresponding author: sitifairuz@kimia.gov.my*

Abstract

Illegal breast augmentation procedures, often involving undisclosed substances, pose significant health risks. This study presents a case where a patient suffered severe complications—swelling, pain, and redness—following an injection of unknown material. Using a handheld Thermo TruDefender FX4580 Fourier Transform Infrared (FTIR) spectrometer, we analyzed the patient's breast fluid aspirate to identify the foreign substance.

FTIR analysis, conducted within the 4000-650 cm^{-1} spectral range, revealed a clear signature of simethicone, a compound commonly used in over-the-counter medications and not intended for breast augmentation. The spectrum exhibited characteristic peaks: a prominent $-\text{CH}_3$ absorption band at 2962 cm^{-1} , indicates the presence of simethicone; a C-Si absorption band at 1258 cm^{-1} ; and Si-O-Si stretching vibrations observed at 1013 cm^{-1} (shoulder) and 796 cm^{-1} . Notably, a peak at 1079 cm^{-1} confirmed the presence of simethicone the mixture of polydimethylsiloxane (PDMS) and silicon dioxide (SiO_2).

These findings demonstrate the efficacy of handheld FTIR as a rapid and non-destructive tool for identifying materials in complex biological samples. The identification of simethicone, a mixture of PDMS and SiO_2 , highlights the dangers of unregulated cosmetic procedures and underscores the importance of robust analytical techniques in forensic toxicology. This study provides valuable insights into the composition of illegal breast fillers, enabling better understanding and management of related complications.

Keywords: breast fillers, polydimethylsiloxane, simethicone, silicone, silicone dioxide, FTIR

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DIFFERENTIATION OF ERASABLE INKS IN FORENSIC QUESTIONED DOCUMENT EXAMINATION: A PILOT STUDY

Teo Chee Hau^{a*}, Nurul Atiqah Mohd Noh^a, Siti Nur Musliha Mohamad Noor^a

^a*Forensic Science Analysis Centre, Department of Chemistry Malaysia, 46661 Petaling Jaya, Selangor, Malaysia.*

**Corresponding author: chteo@kimia.gov.my*

Abstract

Erasable ink pens have gained popularity in Malaysia in recent years. One of the characteristic features of erasable ink is its ability to disappear when exposed to heat, as the colour fades while the ink itself remains on the substrate. When exposed to cold temperature, the ink's colour reappears. This unique property has made the forensic examination of questioned documents involving erasable ink more challenging. This pilot study aimed to differentiate erasable ink pens from different brands of various colours which are available in Malaysian market. A total of 19 erasable ink pens from 5 different brands of black, blue and red colour were used in this study. Specimen handwriting was produced using each respective pen and the inks were examined using Raman Spectral Comparator, a non-destructive method. The result of the analysis showed that 6 black erasable ink pens from 3 different brands can be differentiated into 2 types of spectrum's group. 6 blue erasable ink pens from 5 different brands can be differentiated into 4 types of spectrum's group. However, 3 blue erasable ink pens could not produce complete spectrum due to being highly fluoresce. 4 red erasable ink pens from a single brand can be differentiated into 3 types of spectrum's group. Although there are limited brands that manufacture erasable ink pens, the result of this pilot study showed that the preliminary differentiation of erasable ink pens in Malaysia is feasible.

Keywords: forensic questioned document examination, erasable ink, Raman Spectral Comparator, analysis of ink

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A STUDY ON THE OCCURRENCE OF GENETICALLY MODIFIED MAIZE AND SOYBEAN: AN OVERVIEW AT THE DEPARTMENT OF CHEMISTRY MALAYSIA

Izyan Fartini Md Zuri^{a*}, Sharizah Alimat^a, Noor Shafriza Zainal Azmi^a, Siti Mariam Zhafarina Rusli^a, Noorakmar Jusoh^a, M. Hidayat Rodzihan^a, Azian Murni Ab Ghani^a, Uma Priya Kupusamy^a, Malarvili Ramalingam^a

^a*Biotechnology Division, Drinking Water, Food and Environmental Safety Analysis Centre, Department of Chemistry Malaysia, 46661 Petaling Jaya, Selangor*

^{*}*Corresponding author: izyan.fartini@kimia.gov.my*

Abstract

The widespread use of genetically modified organisms (GMOs) in agriculture and food production has raised global concerns regarding food safety. The Department of Chemistry Malaysia (DOC) serves as the National Food Reference Laboratory (NFRL) and ASEAN Food Reference Laboratory (AFRL), playing a vital role in assisting government agencies with food monitoring and law enforcement in Malaysia, in accordance with the Biosafety Act 2007 and Food Act 1983. This study aims to detect the presence of genetically modified (GM) material in maize and soybean between 2022 and 2024. The laboratory employs molecular approaches, such as polymerase chain reaction (PCR) and real-time PCR (qPCR), for screening seven specific target genes: *35S*, *NOS*, *pat*, *bar*, *cry1A(b)*, *ctp2-cp4epsps*, and *nptII*. Between 2022 and 2024, the laboratory received 352 maize samples and 192 soybean samples. The proportion of maize samples detected with GM material was 29.5% (105 samples) in 2022, 28% (150 samples) in 2023, and 55% (97 samples) in 2024. For soybean, the GM-positive rates were 53% (45 samples) in 2022, 57% (78 samples) in 2023, and 59% (69 samples) in 2024. According to PCR and qPCR results, the most commonly detected target genes in maize and soybean samples were *35S*, *NOS*, *pat*, and *ctp2-epsps*. The data also showed a significant increase in the number of GM-positive samples in both maize and soybean over the years, reflecting a higher importation of GM material into Malaysia. Thus, the development of rapid and sensitive detection methods is crucial for identifying GM material in crops and processed food products. As a scientific service provider, DOC's role is increasingly critical in supporting surveillance agencies to ensure food safety in Malaysia.

Keywords: Real-time PCR, GMO, GM material, Food safety, PCR

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ABANDONED FETAL REMAINS: A CASE STUDY ON FORENSIC DNA PROFILING

**Allia Shahril*, Hasnulhadi Abdullah, Mohd Nazwantul Idlan Mohammad Rushle, Hazwani Hapiz,
Siti Hajar Hussin**

Department of Chemistry, Malaysia

**Corresponding author: allia@kimia.gov.my*

Abstract

Forensic DNA profiling plays a vital role in identifying individuals and establishing biological relationships. In this study, an abandoned fetus was analyzed at the Department of Chemistry, Malaysia, in the absence of a direct maternal reference sample. Four swabs were collected from the fetus's surface, moistened with saline before collection. The fetus was then washed to remove potential contaminants. Finally, a small bone fragment was taken for DNA extraction. All swabs and the fetal bone sample were amplified using the GlobalFiler™ kit and analyzed. STRmix™ probabilistic genotyping software was used to deconvolute the mixture obtained from one of the swabs. The analysis revealed a two-person DNA mixture, with Contributor 1 (30.45%) consistent with the DNA profile obtained from the fetal bone reference sample, and Contributor 2 (69.55%) consistent with the presumed maternal source. Each contributor's profile was observed with 100% component weightage, and at each locus, alleles consistent with a parent-child relationship were identified. The presence of one allele per locus shared between the contributors is indicative of a biological maternal relationship. Likelihood Ratio (LR) analysis is currently being conducted to quantify the statistical support for this relationship across population databases. The updated STRmix™ results strengthen the interpretation that maternal DNA was successfully recovered from a surface swab of the fetus. Future analyses of additional fetal samples are planned to further validate the robustness of this approach in forensic casework. This method allows for the potential inclusion of maternal DNA in forensic databases for future matches, providing a valuable strategy when direct maternal samples are unavailable.

Keywords: Forensic DNA Profiling, Fetal Remains, Maternal DNA, Abandoned Fetus, DNA Mixtures

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QUANTITATIVE ANALYSIS OF SEVEN ANTHELMINTIC DRUGS IN LIVESTOCK AND FISHERY PRODUCTS USING LC-MS/MS

Mi-Ok Kim^{a*}, Ye-Bin Jang^a, Yeong-Ju Jo^a, Gui-Hyun Jang^a

^a*Pesticide and Veterinary Drug Residues Division, National Institute of Food & Drug Safety Evaluation, Osong, Cheongju, Chungcheongbuk-do, 28159, Republic of Korea*

**Corresponding author: kmo95@korea.kr*

Abstract

Anthelmintics are used to treat and prevent diseases in livestock and fishery products and can cause harm to humans if left in food residues. In Korea, the Maximum Residue Limits (MRL) is set for management of residues, but only qualitative test methods are established or presented as individual test methods. Therefore, this study aimed to develop a multi-residue quantitative analytical method for the analysis of seven anthelmintic drugs in livestock (beef, pig, chicken, eggs, milk, and fat) and fishery products (flatfish, eel, and shrimp) using liquid chromatography-tandem mass spectrometry (LC-MS/MS). Each compound was validated at three levels of 0.5, 1, and 2 × MRL or 1, 2, and 10 × LOQ according to the CODEX guidelines (CAC/GL 71-2009). Samples were extracted using the QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) method, and purified using d-SPE (Dispersive-Solid Phase Extraction). The coefficient of determination (R^2) of the matrix-matched calibration curve was higher than 0.99 for all seven components. The recovery was 73.3–118.2% for all target concentrations, and the coefficient of variation (C.V.) was less than 15.2%. This analytical method will increase the efficiency of residue detection and contribute to safety management of livestock and fishery products.

Keywords: Anthelmintics, Liquid chromatography-tandem mass spectrometry, Livestock products, Fishery products,

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FUNCTIONALIZED FULLERENES C₆₀ AND C₇₀ AS NOVEL SORBENTS IN ANALYTICAL CHEMISTRY

Marcin Musielak^{a*}, Maciej Serda^a, Madhav Chavhan^b, Rafal Sitko^a

^a*Institute of Chemistry, University of Silesia in Katowice*

^b*Institute of Chemistry, Faculty of Science, University of Ostrava*

^{*}*Corresponding author: marcin.musielak@us.edu.pl*

Abstract

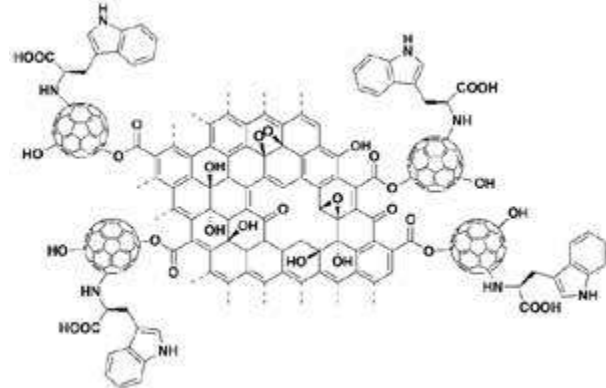
Fullerenes C₆₀ and C₇₀ are promising nanomaterials in analytical chemistry due to their unique structure and high surface area. However, their inherent hydrophobicity limits their direct use in adsorption processes. Functionalization can enhance their metal-binding properties and improve hydrophilicity, but it also increases their solubility in aqueous solutions, making their separation and reuse challenging.¹

To address these challenges, we functionalized C₆₀ and C₇₀ with *L*-tryptophan to improve their affinity for metal ions. To prevent excessive solubility, we anchored them onto graphene oxide and carbon nanotubes, creating stable hybrid materials. Characterization via SEM, TEM, ATR-FTIR, XPS confirmed successful modification. Adsorption studies assessed pH effects, contact time, and ionic strength, with kinetic and isotherm models determining adsorption mechanisms and capacities.

The developed composites: *L*-tryptophan-functionalized fullerene C₆₀ anchored to graphene oxide for Cr, Cu, Hg, Pb adsorption, also fullerenes C₆₀ and C₇₀ attached to carbon nanotubes for selective W and V adsorption, respectively, exhibited high stability and durability in aqueous solutions. Adsorption was dominated by chemisorption, with high metal uptake at sorbent microquantities. The materials maintained excellent selectivity even in the presence of co-existing ions at extreme excess. The materials resisted ionic strength variations and were successfully regenerated for multiple cycles, aligning with green chemistry principles.

These findings confirm that functionalized fullerene-based nanocomposites are highly efficient, selective, and sustainable sorbents, offering promising applications in environmental remediation and analytical chemistry.

Keywords: functionalized fullerenes, adsorption, graphene, carbon nanotubes, analytical chemistry



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A COMPARATIVE INFRARED (IR) SPECTRAL ANALYSIS OF HONDA AND PERODUA AUTOMOTIVE PAINT SAMPLES

Chong Kah Wai^{a,*}, Farah Ad-din binti Nordin^a, Rusyidah binti Abdul Rahim^a

^a*Criminalistics Division, Forensic Science Analysis Center, Department of Chemistry Malaysia, Jalan Sultan, 46661 Petaling Jaya, Selangor Darul Ehsan, Malaysia.*

**Corresponding author: kwchong@kimia.gov.my*

Abstract

This study presents a comparative infrared (IR) spectral analysis of automotive paint samples collected from the basecoats of Honda and Perodua vehicles involved in traffic accident cases commonly received at the laboratory. The analysis reveals notable similarities in paint formulations, with both manufacturers primarily utilizing acrylic and polymethyl methacrylate (PMMA)-based paints. Spectral analysis identified key functional groups, including O-H/N-H stretching ($3370\text{--}3380\text{ cm}^{-1}$), C-H stretching ($2920\text{--}2950\text{ cm}^{-1}$), C=O stretching ($1720\text{--}1730\text{ cm}^{-1}$), aromatic C=C stretching ($1550\text{--}1560\text{ cm}^{-1}$), and C-O stretching ($1150\text{--}1250\text{ cm}^{-1}$), confirming the use of similar polymeric binders and additives in the basecoat layers. These findings highlight the reliance on established paint chemistries for durability, UV resistance, and aesthetic quality. Recommendations for future research include expanding the analysis to incorporate inorganic pigments and additives and broadening the scope to include a wider range of automotive brands. It is hoped that an extensive database of automotive paint compositions could be established that would improve forensic investigations and enhance the accuracy of evidence interpretation.

Keywords: FTIR, automotive, paint, forensic

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DEVELOPMENT AND VALIDATION OF AN ANALYTICAL METHOD FOR MONITORING POLYCYCLIC AROMATIC HYDROCARBONS (PAHS) AND FAT CONTENT IN CACAO MASS (PHILIPPINE *TABLEA*)

Jannelle O. Cristobal^{a,b*}, Charita S. Kwan^a, Benelyn D. Dumelod^b

^a*Research and Analytical Services Laboratory, Natural Sciences Research Institute, University of the Philippines, Diliman 1101 Quezon City, Philippines.*

^b*Department of Food Science and Nutrition, College of Home Economics, University of the Philippines, Diliman 1101 Quezon City, Philippines.*

**Corresponding author: jocrisobal@up.edu.ph*

Abstract

Polycyclic aromatic hydrocarbons (PAHs) are organic compounds formed during thermal processing of cacao and are associated with significant health risks including carcinogenicity. The Philippine cacao industry aims to penetrate the global market with value added products like traditional *tablea*. However, the cacao products need to conform to international food safety standards including international PAH regulatory limits, e.g., EU No. 836/2011. Philippine laboratories lack standardized methods and infrastructure to measure PAHs, necessitating the development of robust analytical protocols. This study developed and validated cost effective analytical procedures for quantifying fat content and nine priority PAHs including Benz[a]anthracene (BaA), Chrysene (Chr), Benzo[b]fluoranthene (BbF), Benzo[k]fluoranthene (BkF), Benzo[e]pyrene (BeP), Benzo[a]pyrene (BaP), Indeno[1,2,3-cd]pyrene (IndP), Dibenzo[a,h]anthracene (DahA), and Benzo[ghi]perylene (BghiP), that are aligned with the AOAC and Eurachem guidelines for validation of analytical methods complying with international safety standards. The validation for fat analysis included recovery studies using cooking oil (n=2) and commercial cacao mass (n=8 samples, duplicate trials). For PAH analysis, a modified method integrating saponification, ultrasonication, liquid-liquid extraction, column chromatography, and solid-phase extraction was used to detect nine PAHs using gas chromatography-mass spectrometry. The validated procedure for fat analysis resulted in a 101% mean recovery and RSD of 1.4%. The commercial samples showed RSD $\leq 4.6\%$ with an average deviation of $\pm 7\%$ from labelled values, complying with the FDA tolerance limits of RSD $\leq 20\%$. Recoveries for PAHs ranged from 90–106% with precision of 5–12% RSD (n=14). Of the analysed samples (n=18), only two exceeded EU thresholds for BaP at 5 $\mu\text{g/kg}$ fat and for $\Sigma 4$ PAHs at 30 $\mu\text{g/kg}$ fat. The validated method will enable local laboratories to measure PAHs in cacao products using accessible techniques while meeting international regulations. Findings highlighted the need for enhanced process controls during roasting to reduce PAH formation, thereby safeguarding public health and promoting the global competitiveness of Philippine cacao products.

Keywords: Polycyclic aromatic hydrocarbons, Philippine *Tablea*, method validation

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ONLINE MONITORING OF INTERFACE REACTIONS BY AMBIENT MASS SPECTROMETRY

Yiyan Yin^a, Xiyang Ge^a, Jin Ouyang^{a,b}, Na Na^{a*}

^aKey Laboratory of Radiopharmaceuticals, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing, 100875, China.

^bDepartment of Chemistry, Faculty of Arts and Sciences, Beijing Normal University, Zhuhai, 519085, China.

*Corresponding author: nana@bnu.edu.cn

Abstract

With the distinctive physicochemical characteristics of the interfaces between different phases, interfacial reactions have consistently garnered significant attention. Investigation of interface reactions is crucial for revealing and understanding of novel reactions, further facilitating the development of highly efficient reactions. While these reactions were employed at the unique interfaces, greatly challenges the reaction examinations. Ambient mass spectrometry (AMS) enables direct capture and identification of intermediates in the reaction systems without or with less pretreatment, holding significant advantages in investigating reaction mechanisms in complex systems. Various AMS methods have been systematically developed for monitoring and investigation of diverse reactions, including enzyme-catalyzed reactions, photocatalytic reactions, and even some biochemical processes during a certain therapy.¹⁻³ Based on the monitoring by AMS, some key intermediates were captured and identified during the reaction process. Thereby, the reaction mechanisms were investigated and deduced based on the comprehensive characterizations and theoretical calculations. Consequently, AMS will exhibit distinct benefits in monitoring and investigating the interfacial reactions, such as the gas-liquid and solid-liquid interface reactions.

Herein, to examine the gas-liquid interface reactions, a model of the photochemical conversions in a droplet was selected for the examination by AMS. As investigated, under visible-light irradiation, the pollutant model of 4-bromo-1,2-phenylenediamine (BP) is rapidly converted into several secondary pollutants in droplets, while no significant conversion is observed in the bulk system. Thereby, to investigate the photochemical conversions in the droplet, a single droplet contains BP was kept on a Y-shaped Cu electrode for the in situ electrospray ionization.⁴ Different pollutant conversions at the water–air interface and inner droplet were recorded by the dynamic monitoring via MS detections layer-by-layer. By examining the observed intermediates, photochemical mechanisms across the water–air interface were proposed. Besides, the solid-liquid interface reactions were also examined with the visible light-catalyzed indole cyclization reaction within a confined space of the needle tip as a model.⁵ As revealed, the silicon hydroxyl groups generated on the needle tip surface can enhance the enrichment of Ru catalyst on the solid-liquid interface, maintaining highly efficient photocatalytic conversions at the interface. The efforts would enlarge applications of AMS into more specific reaction examinations.

Keywords: ambient mass spectrometry, online monitoring, interface reactions, reaction intermediates, mechanism studies

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INVESTIGATING SOLUBILITY AND STABILITY IN DEVELOPING STANDARD GAS MIXTURES FOR INSULATING OIL APPLICATIONS

Hadi Fauzi^{a*}, Manal Ismail^{b*}

^a *Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia,
43600 UKM Bangi, Selangor, Malaysia.*

^b *TNB Labs (EtODS), TNB Research, No.1 Lorong Ayer Itam, Kawasan Institusi Penyelidikan dan Latihan Bangi,
43000 Kajang, Selangor, Malaysia*

**Corresponding author: hadi.fauzi@gmail.com*

Abstract

The calibration of Dissolved Gas Analysis (DGA) for transformer fault detection relies on gas-in-oil standards, yet commercial standards face challenges in accuracy, stability, and reproducibility due to short shelf life, supply chain delays, and incompatibility with diverse transformer oils. This study develops a repeatable, stable in-house gas-in-oil standard while analysing container material effects, oil properties, and temperature influences on gas solubility and diffusion. The in-house standard is validated against the Morgan Schaffer Certified Reference Material (CRM).

The methodology integrates Henry's Law, the Bunsen Absorption Coefficient, the Arrhenius Equation, Stokes–Einstein Relation, Fick's Law, and Permeation Theory to assess gas solubility, stability, and retention. Gas Chromatography (GC) was used at 10 ppm, 100 ppm, and 500 ppm concentrations to compare with Morgan Schaffer's True North standard. Additionally, oil property correlation analysis was conducted to evaluate viscosity, density, and polarity effects on gas solubility.

Validation against Morgan Schaffer's standards showed strong agreement for six key fault gases (H_2 , CH_4 , C_2H_4 , C_2H_6 , C_2H_2 , CO), with recovery rates of 90.9–109.1%. Glass containers exhibited the lowest standard deviation, proving optimal for long-term gas retention. Temperature studies established optimal storage conditions, while oil property analysis confirmed that calibration oil must match transformer oil.

This study establishes a validated, reproducible methodology for preparing gas-in-oil standards, confirming that the in-house standard is a cost-effective, stable, and reliable alternative for DGA calibration and transformer maintenance.

Keywords: Dissolved Gas Analysis; Standard Gas-in-Oil; Insulating Oil; Transformer; Gas-Chromatography

RISK ANALYSIS OF HEAVY METAL CONTAMINATION ON PUBLIC HEALTH IN THE AQUATIC AREA OF THE CITARUM RIVER, WEST JAVA PROVINCE, INDONESIA

Satriani Aga Pasma^{a,*}, Retno Wulandari^a, Muhayatun Santoso^b

^aNational Intelligence College (Sekolah Tinggi Intelijen Negara), Bogor, Indonesia

^bNational Research and Innovation Agency (BRIN), Bandung, Indonesia.

*Corresponding author: satriani.ap@gmail.com; satriani.aga.pasma@stin.ac.id

Abstract

The Citarum River is one of the primary water sources in Indonesia, playing a crucial role in the livelihoods of surrounding communities, including residential areas, agriculture, fisheries, tourism, hydroelectric power generation, and as a discharge site for industrial activities contributing to pollution. This pollution includes heavy metals such as arsenic (As), cadmium (Cd), iron (Fe), manganese (Mn), and zinc (Zn). This study aims to quantitatively analyze the contamination profile of heavy metals in the upstream, middle, and downstream sections of the Citarum River, West Java. The analysis was conducted using an Inductively Coupled Plasma Mass Spectrometer (ICP-MS), and the health risk assessment was carried out using the Contaminant Daily Intake (CDI), Hazard Quotients (HQ), and Excess Lifetime Cancer Risk (ELCR) approaches. Method validation was performed to ensure the reliability of the analytical method, evaluating parameters such as linearity, precision, intermediate precision, accuracy, and detection and quantification limits (LOD and LOQ). The results showed that the method met the required criteria with $R^2 > 0.995$, %RSD $< 5.30\%$, recovery rates ranging from 40% to 120%, and metal concentrations detected within the limits of detection and quantification. The findings revealed that Cd, Fe, and Mn concentrations exceeded the permissible limits in the middle section of the river, with concentration ranges of 0.000034 – 0.001360 mg/L for Cd, 0.0420 – 0.4180 mg/L for Fe, and 0.0101 – 0.0215 mg/L for Mn. Zinc (Zn) concentrations exceeded the permissible limits across all sections—upstream, middle, and downstream—with ranges of 0.0021 – 0.0092 mg/L, 0.0017 – 0.0234 mg/L, and 0.0007 – 0.0082 mg/L, respectively. The HQ value for arsenic (As) in the middle section exceeded 1 for the age group 0-59 months, indicating a potential non-carcinogenic health risk. In addition, ELCR values exceeded 10^{-4} for arsenic (As) across all age groups and locations, and for cadmium (Cd) in the middle section for the age groups 0-59 months and 5-12 years, indicating significant carcinogenic health risks. This study highlights the critical importance of early detection and early warning systems and supports government efforts to prevent and mitigate the impact of heavy metal exposure on public health and the environment in Indonesia.

Keywords: Inductively Coupled Plasma Mass Spectrometer (ICP-MS), Health Risk Assessment, Citarum River Pollution, Heavy Metal Contamination, Excess Lifetime Cancer Risk.

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DETERMINATION OF BIOGENIC AMINES (CADAVERINE, PUTRESCINE, TYRAMINE, HISTAMINE) IN MILK AND WINE USING HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC)

Anna Salimova^{a,*}, Alexandra Vasilyeva^b

^a *Disinfectology Institute of F.F. Erisman FSCH of Rospotrebnadzor, Moscow, Russia*

^b *RTU MIREA, Moscow State University of Fine Chemical Technologies named after M.V. Lomonosov, Moscow, Russia*

**Corresponding author: monika94@bk.ru*

Abstract

Biogenic amines (BAs) are nitrogen-containing compounds formed as a result of microbial decarboxylation of amino acids. In foods such as milk and wine, BAs (cadaverine, putrescine, tyramine, histamine) can accumulate during storage and fermentation. High concentrations of BAs, especially histamine and tyramine, pose health risks to consumers, causing allergic reactions and headaches. Therefore, monitoring their levels in food is an important task^{1,2}.

The determination of biogenic amines in food is an important issue today. The direct determination of the selected amines is extremely difficult because, due to their chemical structure, amines do not absorb in the UV region of the spectrum and the complex protein structure of milk makes their extraction difficult.

In this work, a method for the determination of biogenic amines by high-performance liquid chromatography with pre-derivatisation has been developed. The interaction of the amines with the derivatising agent tosyl chloride was studied and a method for the preliminary extraction of BAs from milk, red, white and rosé wine was developed. The best separation of the components was achieved using an Acclaim 4.6×150 mm C8, 5 µm analytical column in gradient elution mode at a flow rate of 1 ml/min.

Keywords: biogenic amines, high-performance liquid chromatography, food, derivatization

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CHALLENGES AND STRATEGIES IN DEVELOPING ELECTROCHEMICAL GLUCOSE BIOSENSOR BASED ON GOLD NANOSTRUCTURES

Almira Ramanaviciene^{a,*}, Katazyna Blazevic^a, Kristina Sobol^a, Asta Kausaite-Minkstiniene^a

^a NanoTechnas – Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Lithuania

*Corresponding author: almira.ramanaviciene@chf.vu.lt

Abstract

As the number of people with diabetes increases every year, sensitive, selective, easy-to-use, and fast methods for the determination of glucose levels in the blood are in high demand. Electrochemical biosensors based on immobilized enzymes have received significant attention due to their exceptional selectivity, low limit of glucose detection, and high sensitivity. The performance of such biosensors can be improved through the application of various nanomaterials [1-3]. Gold nanostructures deposited on the electrode surface increase the electrochemically active surface area and conductivity, thus improving the electron transfer and the analytical performance of the biosensor. The optimal surface concentration and proper immobilization of the enzyme on the gold nanostructures are critical factors affecting the performance of the biosensor [4].

In this study, the impact of gold nanostructures electrochemically synthesized on a graphite rod electrode, as well as the method of enzyme glucose oxidase immobilization, were evaluated in the development of reagentless glucose biosensors. The redox mediator tetrathiafulvalene was applied for the modification of gold nanostructures synthesized on the electrode. Under optimal conditions, the biosensor exhibited a linear current response to glucose concentrations ranging from 0.2 to 20 mmol L⁻¹, with the detection limit of 0.028 mmol L⁻¹. The performance of the developed biosensor was evaluated in a blood serum sample and compared with other reagentless electrochemical glucose biosensors based on gold nanomaterials.

Keywords: glucose biosensor, gold nanostructures, glucose oxidase, electrochemical methods

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EFFECT OF DIFFERENT HYDROPHILIC LIPOPHILIC BALANCE VALUE ON STABILITY OF SACHA INCHI OIL EMULSION

Nabilah Hauzin^{a*}, Nurul Lina Mohamad^a, Ros Haniza Borhan^a,

^aFeed & Industrial Technology, Downstream Technology, FGV R&D Sdn Bhd., FGV Innovation Centre, 71760

Bandar Enstek, Negeri Sembilan, Malaysia.

**Corresponding author: nabilah.hauzin@fgvholdings.com*

Abstract

Sacha inchi oil is gaining popularity among researchers due to its outstanding health advantages and unique balance of omega-3, 6, and 9 essential fatty acids, which are uncommon in other vegetable oils. However its high content of polyunsaturated fatty acids makes it susceptible to oxidation, which can lead to off-flavors and nutrient degradation. To overcome the limitations of sachu inchi oil, emulsion was employed. This study evaluated the influence of various hydrophilic-lipophilic balance (HLB) values on the stability and creaming index of sachu inchi oil emulsion, with Tween 20 used as hydrophilic surfactant and Span 80 as hydrophobic surfactant. The stability and creaming index of the emulsion were examined over a 28-day period at different HLB values. With the lowest creaming index and the maximum stability throughout the observation period, the ideal HLB value of sachu inchi oil emulsion is 8.5. This work provides valuable insights into the HLB value and emulsion properties of sachu inchi oil, which are useful for cosmetic, food and pharmaceutical applications.

Keywords: Sachu Inchi Oil, Hydrophilic-lipophilic Balance Value, Emulsion, Stability

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MID-INFRARED CAVITY RING-DOWN SPECTROSCOPY FOR SPECTRAL REFERENCE DATA AND ULTRA-TRACE DETECTION OF GAS SPECIES

D. Michelle Bailey*, Eisen C. Gross, Joseph T. Hodges, and Adam J. Fleisher

National Institute of Standards and Technology, Gaithersburg, MD, USA

**Corresponding author: michelle.bailey@nist.gov*

Abstract

Cavity ring-down spectroscopy (CRDS) is a stable, reproducible, and sensitive technique that enables metrology-grade measurements of gaseous species. By leveraging this SI-traceable technique with gravimetrically prepared gas samples we can provide spectroscopic reference data that describe fundamental physical attributes of gas phase molecules. These parameters, including molecular transition intensity, are necessary for accurate spectroscopic modelling and can impact the accuracy of experimental retrievals. Here we will present ultra-precise mid-infrared CRDS measurements enabled by state-of-the-art amorphous-crystalline mirrors [1]. Recent experimental results for a carbon monoxide transition intensity in the fundamental band will be discussed. Further, we will present initial results that leverage cutting-edge sensitivity to quantify trace amounts of constituent species (e.g., CO and N₂O) in high-purity balance gases used in industry.

Keywords: optical spectroscopy, cavity ring-down spectroscopy, mid-infrared

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DEVELOPMENT OF A μ -SOLID PHASE EXTRACTION DEVICE FOR EFFICIENT ENVIRONMENTAL POLLUTANT ANALYSIS IN WATER

Muhammad Nur' Hafiz Rozaini^a, Noorfatimah Yahaya^b, Muggundha Raoov Ramachandran^c

^aPRIMOChem Sdn Bhd, Lot 67 – 70 Jalan Industri 4/2, Gopeng Light Industrial Park, 31600 Gopeng, Perak, Malaysia.

^bDepartment of Toxicology, Advanced Medical and Dental Institute (AMDI), Universiti Sains Malaysia, 13200 Bertam, Penang, Malaysia.

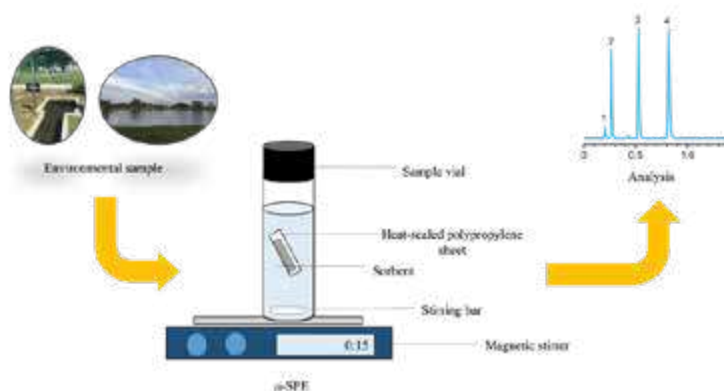
^cDepartment of Chemistry, Faculty of Science, Universiti Malaya, Kuala Lumpur, Malaysia

*Corresponding author: m.n.hafizrozaini93@gmail.com

Abstract

The detection of endocrine disruptor compounds (EDCs) in water requires advanced sample preparation techniques to achieve high sensitivity and selectivity. This study introduces a micro-solid phase extraction (μ -SPE) device designed to enhance extraction efficiency through the integration of tailored sorbents. The μ -SPE device was optimized for key parameters, including extraction efficiency, detection limits, and enrichment factors, across various environmental water samples. The developed method demonstrated excellent selectivity, rapid adsorption kinetics, and high recovery rates, with enrichment factors reaching up to 82-fold. The μ -SPE device exhibited strong performance across different water matrices, including wastewater, river water, and tap water, with low detection limits ranging from 0.27 to 0.92 $\mu\text{g L}^{-1}$. Recovery rates between 78.5% and 105.5% manifested the reliability of the method for real sample analysis. Furthermore, the μ -SPE approach significantly reduced solvent consumption, aligning with green chemistry principles while maintaining high analytical precision. This study highlights the potential of μ -SPE as an efficient, cost-effective, and environmentally friendly tool for monitoring trace pollutants in water.

Keywords: Micro-solid phase extraction, endocrine disruptor compounds, water analysis, environmental monitoring



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DETECTION OF ADULTERANT IN *Aloe barbadensis* MILLER GEL USING FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR) WITH CHEMOMETRICS

Su-Yen Chen^a, Khye Er Loh^{a*}, Ghim Hock Ong^b

^aDepartment of Bioscience, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Klang, Setapak, 53300 Kuala Lumpur, Malaysia

^bFaculty of Health and Life Sciences, INTI International University, Persiaran Perdana BBN, Putra Nilai, 71800 Nilai, Negeri Sembilan, Malaysia

*Corresponding author: lohke@tarc.edu.my

Abstract

Aloe barbadensis Miller, commonly known as aloe vera, is widely used across various industries, from cosmetic to pharmaceuticals, due to its significant anti-inflammatory properties. Although adulterating aloe vera gel with cheaper substitutes such as maltodextrin does not raise safety concerns, it presents notable challenges to the product's quality and efficacy. This study investigates aloe vera gel adulteration using Fourier Transform Infrared Spectroscopy (FTIR) coupled with chemometrics techniques, particularly Principal Component Analysis (PCA), Partial Least Square (PLS), and Partial Least Squares Discriminant Analysis (PLS-DA). The results showed that the PCA model effectively discriminates between pure aloe vera gel, adulterated samples, and retail aloe vera gel. Notably, brand A of the retail aloe vera gel clusters with aloe vera gel adulterated with 2% maltodextrin. PLS-DA models further revealed that retail aloe vera gel from brand A might be adulterated with low level of maltodextrin, while brands B and C may contain ethanol. The PLS biplot provides insight into the correlation between different aloe vera gels and the Y-variables. It shows that pure aloe vera gel exhibits higher anti-inflammatory activity than the adulterated samples, implying that the presence of maltodextrin may reduce its anti-inflammatory potential. The Partial Least Squares Regression (PLSR) model, based on anti-inflammatory activity as the Y variable, demonstrated high accuracy ($R^2 = 0.995$) and good predictive ability (RMSEE = 0.0133 and RMSEcv = 0.0995). This approach offers a reliable analytical method for detecting adulterants in aloe vera gel and ensuring product authenticity in the market, thereby safeguarding both its quality and effectiveness.

Keywords: Adulteration, FTIR, PCA, PLS, maltodextrin

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CALCIUM NANOMODULATORS FOR DUAL-MODE CANCER THERAPY VIA IN SITU MINERALIZATION AND MITOCHONDRIAL DYSFUNCTION

Yingxia Miao, Weicai Wang*, Zongjin Qu*

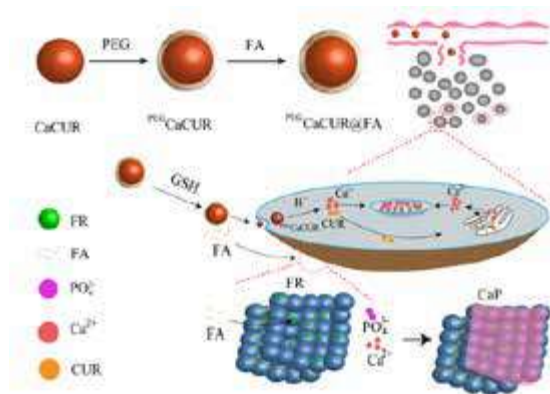
Shandong Key Laboratory of Tumor Imaging Equipment Development and Integrated Diagnosis and Treatment Technology, Linyi University, Linyi 276005, China

*Corresponding author: weicaiwang012@163.com; quzongjin@lyu.edu.cn

Abstract

Calcium (Ca^{2+}) nanomodulators, such as calcium carbonate nanoparticles, have emerged as promising agents for cancer therapy by inducing Ca^{2+} overload. However, their potential in combination therapies targeting mitochondrial dysfunction and in situ mineralization remains underexplored. This study aims to develop a multifunctional Ca^{2+} nanoregulator (PEGCaCUR@FA) incorporating curcumin (CUR) and folate (FA) to synergize mitochondrial Ca^{2+} overload and tumor mineralization for enhanced anticancer efficacy. PEGCaCUR@FA was synthesized via a one-pot strategy, encapsulating CUR within CaCO_3 nanoparticles. Surface modification with polyethylene glycol (PEG) improved dispersibility, while FA was conjugated via a disulfide linker for tumor targeting. The nanoparticles were characterized for pH/GSH-responsive degradation, FA release, and dual-mode imaging capabilities. Mechanistic studies evaluated mitochondrial Ca^{2+} accumulation, biomimetic mineralization, and apoptosis induction. In the tumor microenvironment, PEGCaCUR@FA released FA via GSH-triggered linker cleavage, enabling folate receptor-mediated cellular uptake. Acidic conditions degraded CaCO_3 , releasing Ca^{2+} and CUR. CUR amplified cytoplasmic Ca^{2+} by inhibiting efflux and promoting endoplasmic reticulum release, leading to mitochondrial Ca^{2+} overload, dysfunction, and caspase-3 activation. FA facilitated in situ mineralization by nucleating calcium phosphate on cell membranes, disrupting cellular integrity. Ultrasound enhanced Ca^{2+} influx and nanoparticle internalization. PEGCaCUR@FA also exhibited photoacoustic/fluorescence imaging properties, enabling real-time tracking. This nanoplatform integrates mitochondrial targeting and in situ mineralization, offering a dual-mode therapeutic strategy with imaging-guided precision. Its synergistic design overcomes limitations of conventional therapies, highlighting potential for translational cancer treatment.

Keywords: calcium nanomodulators, in situ mineralization, mitochondrial dysfunction, curcumin, folate targeting



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NEAR-INFRARED OPTOGENETIC UPCONVERSION NANOPARTICLE COMPLEX FOR HIGH-EFFICIENCY IN SPLIT-CAS9 SYSTEM FOR GENE EDITING

Yuqi Zhang^a, Mengmeng Li^a, Yan Zhang^a, Xinli Shi^a, Yujun Sun^a, Chunping Ge^a, Xinyue Song^{b*}, Pengfei Shi^{b*}

^aCollege of Chemistry and Chemical Engineering, Linyi University, Linyi 276005, China

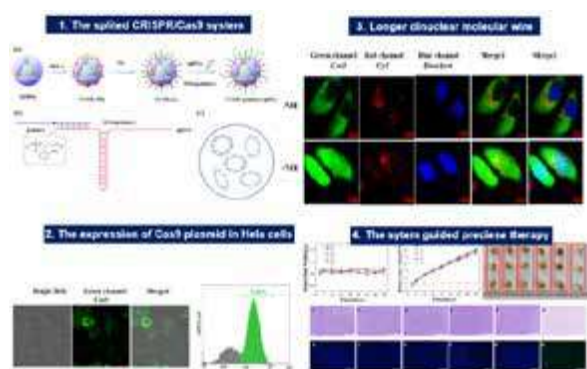
^bShandong Key Laboratory of Tumor Imaging Equipment Development and Integrated Diagnosis and Treatment Technology, Linyi University, Linyi 276005, China

*Corresponding author: songxinyue428@163.com (X. Y. Song); shipengfei913@163.com (P. F. Shi)

Abstract

As a renovator in the field of gene editing, CRISPR/Cas9 plays an essential role in advancing next-generation gene therapy owing to its simplicity and precision. However, this potential faces significant challenges primarily stemming from the difficulty in efficiently delivering large-sized genome edition system (including Cas9 protein and sgRNA) into targeted cells and spatiotemporally controlling their activity in vitro and in vivo. Herein, we developed a near-infrared light-controlled CRISPR/Cas9 activity system comprised three key components: (a) upconversion luminescent nanoparticles NaYF₄:Yb,Tm@NaYF₄ capable of emitting intense UV light upon 980 nm laser irradiation; (b) DNA, comprised of UV-responsive cleavable DNA with pc-linker, are employed for attaching to sgRNA targeting the cancer therapeutic gene polo-like kinase 1 (PLK-1) and enabling spatiotemporally controlled gene editing through UCNPs-mediated photo-conversion; (3) A plasmid that can be transfected to express Cas9 protein in cancer cells. By delivering the Cas9 plasmid and sgRNA separately, a split Cas9 gene editing platform was created, which avoided the degradation caused proteases during the direct delivery of Cas9 protein and sgRNA, as well as the risk of random integration of the all-in-one plasmid, greatly the efficiency of in vivo gene editing and significantly inhibiting tumor growth. Notably, controlling the CRISPR/Cas9 gene editing by controlling the sgRNA simplifies the workflow and provides new ideas for controllable on-demand treatment of tumors. The obtained Cas9 plasmid could be well expressed in Hela cells with the transfection efficiency of around 76.42%, and the tumor inhibition rate is 82.7%. The developed optogenetic nanosystem was controllable and activatable, showed decreased side-effects compared with the conventional “always-on” therapy method and provided new ideas for controllable on-demand treatment of tumors.

Keywords: upconversion, CRISPR/Cas9, optogenetic, gene editing, tumor



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SYNTHESIS OF MOLYBDENUM NITRIDE AND NICKEL NITRIDE AS MICROELECTRODE MATERIALS FOR HYDROGEN GAS SENSING

Daniel Rashidi^a & Saiful Arifin Shafiee^{a*}

^aInternational Islamic University Malaysia (IIUM),

*Corresponding author: sabs@iium.edu.my

Abstract

As the world is transitioning to a hydrogen economy, hydrogen sensors play crucial role for early gas leak detection, ensuring public safety and equipment protection. The reliance on noble metals such as platinum (Pt) and palladium (Pd) in hydrogen sensors are limited by their scarcity and high-cost, leading to increased production costs while hindering widespread application. Transition metal nitride (TMN) exhibits on par catalytic ability to noble metals given the modification in the electronic band gap structure. In this study, molybdenum nitride, (Mo_2N) and nickel nitride (Ni_3N) microwire of 25-micron diameter were cut into several 1-cm in length and synthesised via temperature programmed ammonolysis in plug furnace reactor for 8 hours at 800 °C and 1000 °C, respectively. SEM imaging reveals the nitrided metals porous surface structure which increase the effective surface area for hydrogen detection while XRD analysis successfully confirmed the formation of hexagonal Ni_3N and cubic Mo_2N . This study investigates the electrochemical behaviour of Mo_2N and Ni_3N microelectrodes compared to molybdenum (Mo), nickel (Ni), Pt, and Pd microelectrodes in 0.1 M potassium chloride (KCl) solution in the presence of 10 mM of hexamine ruthenium (III) chloride redox mediators. Results show that both Mo_2N and Ni_3N display improved electrochemical performance than their pristine forms. However, when it comes to electrochemical characterisation in the presence of single electron transfer redox mediators in aqueous solutions, the redox processes seem to proceed with kinetically controlled reaction. However, the electrochemical behaviour of these electrodes towards the redox process of dissolved hydrogen gas in aqueous solutions are then probed. The study should be able to enlighten researchers on the possibility of metal nitride materials being used for hydrogen gas detection system which could be an alternative to the existing materials used for the sensors.

Keywords: molybdenum nitride, nickel nitride, hydrogen gas, sensors, and electrochemistry

APREPITANT-LOADED PLGA NANOPARTICLES FOR LUNG CANCER: PHARMACEUTICAL AND ANTI-CANCER PERSPECTIVES

Elif Kaya Tilki^a, Selin Engür Öztürk^b, A. Alper Öztürk^{c*}

^aAnadolu University, Faculty of Pharmacy, Department of Pharmacology, Eskisehir, Türkiye.

^bPamukkale University, Tavas Vocational School of Health Services, Department of Pharmacy Services, Denizli, Türkiye.

^cAnadolu University, Faculty of Pharmacy, Department of Pharmaceutical Technology, Eskisehir, Türkiye.

*Corresponding author: aaozturk@anadolu.edu.tr

Abstract

Polymeric nanoparticle-based drug delivery systems have gained attention in cancer therapy due to their ability to improve drug solubility, stability, and tumor-specific accumulation. PLGA (poly(lactic-co-glycolic acid)) nanoparticles, approved by both the FDA and EMA, are particularly promising due to their biocompatibility, biodegradability, and controlled drug release properties. Lung cancer is the second most common cancer type worldwide and remains a leading cause of cancer-related mortality. Despite advances in targeted therapies, chemotherapy remains a primary treatment strategy, though its efficacy is limited by severe side effects and frequent dosing. Innovative drug delivery systems are being developed to enhance therapeutic efficacy while reducing systemic toxicity.¹ In Aprepitant, an FDA-approved neurokinin-1 (NK-1) receptor antagonist used for chemotherapy-induced nausea and vomiting, was encapsulated into PLGA nanoparticles via the nanoprecipitation method. These nanoparticles were characterized according to ICH and FDA guidelines, ensuring compliance with regulatory standards for cancer therapeutics. The anti-cancer potential of aprepitant-loaded nanoparticles was evaluated in A549 human lung cancer cells using real-time cell analysis. Migration and invasion assays were performed in a co-culture model with M2c-polarized THP-1 macrophages to assess their anti-metastatic effects.²⁻⁴ The IC₅₀ values of free aprepitant and aprepitant-loaded nanoparticles were 126 µg/ml and 105 µg/ml at 24 hours, and 107 µg/ml and 93.4 µg/ml at 48 hours, respectively. Migration increased by 40.44% in the M2c group but was reduced by 11.38% with aprepitant and 31.72% with aprepitant-loaded PLGA. Invasion rates rose by 59.72% in the M2c group but decreased by 35.47% and 64.99% with aprepitant and aprepitant-loaded PLGA, respectively. Aprepitant-loaded PLGA nanoparticles significantly reduced migration and invasion in lung cancer cells, demonstrating their potential to enhance anti-cancer efficacy while minimizing side effects. This work has been supported by Anadolu University Scientific Research Projects Coordination under grant number BGT-2024-2344 / ID: 2344.

Keywords: Aprepitant, Nanoparticles, PLGA, Pharmaceutical analysis.

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ANALYSIS OF SUGAR CONTENT IN READY-TO-DRINK SUGAR-SWEETENED BEVERAGES USING UHPLC-ELSD

Loo Poh Ling*, Muhamad Shafudin Saad, Lailatul Nazira Topani, Mohd Irwan Wahab, Norfadila binti Mohammad

Industry and Customs Tariff Analysis Centre, Department of Chemistry Malaysia

**Corresponding author: loopohling@kimia.gov.my*

Abstract

As part of efforts to enhance the quality of life for the community and address the rising concerns of obesity and non-communicable diseases (NCDs) among Malaysians, the Minister of Finance, in the presentation of Budget 2019, announced the implementation of an excise duty, commonly referred to as a “sugar tax” on ready-to-drink sugar-sweetened beverages. Therefore, a rapid and reliable method for quantifying five natural sugars, namely fructose, glucose, sucrose, maltose and lactose in ready-to-drink sugar-sweetened beverages has been developed using Ultra High Performance Liquid Chromatography with Evaporative Light Scattering Detector (UHPLC-ELSD). Three categories of beverages were analyzed: non-alcoholic beverages, animal milk-based beverages and fruit juices. Chromatographic separation was achieved using a LC-NH2 column at 35 °C, with a flow rate of 1.8 mL/min and a mobile phase consisting of 80% acetonitrile and 20% water. The developed method demonstrated good linearity with an $R^2 > 0.999$. The limits of detection (LOD) and limits of quantification (LOQ) for the five sugars were 0.02% and 0.05% respectively. The method demonstrated good precision, with a relative standard deviation (RSD) of less than 2.0% and satisfactory accuracy, with average recovery ranging between 104% and 119%. In conclusion, the developed UHPLC-ELSD method is reliable for the simultaneous detection and quantification of the above-mentioned sugars in ready-to-drink sugar-sweetened beverages.

Keywords: sugar content, beverages, UHPLC-ELSD

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DETERMINATION OF CERAMIDE AND SPHINGOID BASES IN COSMETIC PRODUCTS BY GC-MS WITH TRIMETHYLSILYLATION DERIVATIZATION

Shi Ngar Pang^a, Norsyariza Abd Aziz^a, Chung Lee Yee^a, Khan Loon Ng^{a*}, Mong Sah Toh^a

^aWinnox Cosmeceutics, No 7 Persiaran Subang Permai, Taman Perindustrian Subang, 47610 Selangor, Malaysia

*Corresponding author: ng.khanloon@wipro-unza.com

Abstract

Human skin is an effective physical barrier that prevents water loss and keeps out harmful substances and microorganisms. The stratum corneum, located in the outermost layer of the skin, plays an important role as a component of the skin barrier. It is embedded with multilamellar lipid membranes, which are composed of cholesterol, free fatty acids and ceramides (CERs)¹, with the latter comprising 30–40% of the total stratum corneum lipids by mass. Changes in CERs level and lipid composition in stratum corneum can be associated with dry skin and various skin disorders. Therefore, various skin care formulations had incorporated CERs to replenish the decreased CERs levels and improve the skin disorder with barrier defects. To identify the CERs composition in skin care formulation, comprehensive lipidomic profiling analysis is important to assure the bioavailability of the molecules. In this studies, gas chromatography-mass spectrometry (GC-MS) coupled with trimethylsilylation (TMS) derivatization was developed to identify and quantify the wide range of non-volatile lipidomic species, including ceramides and sphingoid bases. Due to their volatility and thermal stability, TMS derivatization was used to provide high separation efficiency and to increase the detectability of CERs. The developed method showed an acceptable limit of quantification of 1.732 $\mu\text{g mL}^{-1}$ and a calibration curve with a correlation coefficient of above 0.999, covering a concentration range of 3 $\mu\text{g mL}^{-1}$ to 100 $\mu\text{g mL}^{-1}$. Six ceramides and two sphingoid bases were successfully separated, identified and quantify. The method was validated with 2 market samples, and to ensure method reliability, spike analyses of Ceramide III and Ceramide IIIB were performed, with recoveries of above 89% and 82%, respectively. This approach provides insight into lipidomics research, contributing to deeper understanding of lipid functions, the effect of skin disorders, and the development of skincare formulations for topical application of ceramides and sphingoid bases.

Keywords: Lipidomics, gas chromatography-mass spectrometry (GC-MS), trimethylsilylation, ceramides (CERs), sphingoid bases

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PERSISTENCE OF CYROMAZINE, TEBUCONAZOLE, AND TRIFLOXYSTROBIN RESIDUES IN RED SHALLOT LEAVES (*Allium cepa* var. *aggregatum*)

Christine Jinang^{a*}, Lai Lee San^a, Jisia Jimbau^a, Ngan Chai Keong^b, Margaret Abat^a, Maclin Dayod^a

^aAgriculture Research Centre Semongok, Department of Agriculture Sarawak, KM20, Borneo Heights Road, 93250 Kuching, Sarawak

^bSoil, Water & Fertilizer Research Centre, Malaysian Agriculture Research & Development Institute, MARDI Headquarter, Persiaran MARDI-UPM, 43400 Serdang, Selangor

*Corresponding author: christj3@sarawak.gov.my

Abstract

In Malaysia, there is no recommended pesticide for leafy herbs and only one fungicide registered for use on shallots, which is chlorothalonil. Growers of some minor crops especially leafy herbs are facing limited legal access to pesticides because of the lack of interest from the agrochemical manufacturers in conducting studies due to the restricted target coverage for pesticide use on these minor crops. Therefore, a study was conducted to assess the selected pesticides residues in red shallot leaves grown by farmer at Siburan, Serian, Sarawak. Cyromazine (75 g/ha, 150 g/ha and 300 g/ha), and a combination of tebuconazole and trifloxystrobin (50 g/ha, 100 g/ha and 200 g/ha) were applied to red shallots cultivated under the recommended agronomic practices. The plants were sampled at periodic intervals over 14 days after being treated with the pesticides. The cyromazine, tebuconazole, trifloxystrobin and its metabolite in the red shallots leaves were determined using a liquid chromatography equipped with a triple quadrupole spectrometer. The cyromazine and tebuconazole residues were observed up to 14 days after application for all of the treatments at concentration levels ranged from 0.005 mg/kg to 0.041 mg/kg. Meanwhile, the trifloxystrobin and its metabolite, trifloxystrobin acid residues were observed up to 7 days after application and reached below the quantification level (0.005 mg/kg) at 14 days. Our findings suggest that a proper pre-harvest interval shall be observed.

Keywords: Pesticides, accumulation, degradation, LC-MSMS, red shallot leaves

CLASSIFICATION OF KIMCHI CONSUMED IN SOUTH KOREA BY COUNTRY OF ORIGIN USING k -NEAREST NEIGHBORS BASED ON ELEMENTAL COMPOSITION

Yonghoon Lee^{a,*}

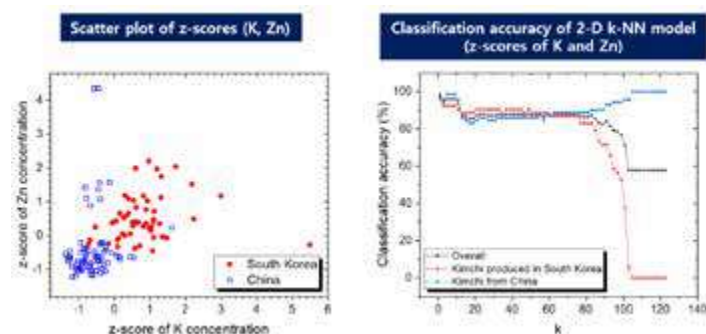
^aDepartment of Energy and Chemical Engineering, Mokpo National University, Republic of Korea.

*Corresponding author: yhlee@mokpo.ac.kr

Abstract

This study explores the use of k -nearest neighbors (k -NN) modeling to distinguish between cabbage kimchi produced in South Korea and China. A total of 125 samples were collected from South Korean markets, comprising 53 domestic and 72 Chinese-imported kimchi. Elemental analysis of 15 elements (Ca, K, Mg, Na, P, S, Al, Ba, Cu, Fe, Mn, Sr, Zn, B, and Si) was performed using inductively coupled plasma optical emission spectroscopy (ICP-OES). Major elements such as Ca, K, Mg, Na, P, and S were detected at concentrations between 1,000 and 50,000 mg/kg, while the remaining elements ranged from 1 to 50 mg/kg. Based on one-dimensional k -NN classification accuracy, K, Mg, and Zn were identified as the most effective elements for multi-dimensional modeling. However, direct combination of these variables, due to differing concentration scales, did not enhance classification performance. Applying z -score normalization effectively equalized variable influence and improved model synergy. Among the z -score-based models, a two-dimensional k -NN using K and Zn achieved the highest classification accuracy of 98% at $k = 1$. These findings highlight the importance of both thoughtful variable selection and proper data preprocessing. Our ICP-OES-based method was compared with previously reported approaches using laser-induced breakdown spectroscopy (LIBS)¹ and inductively coupled plasma mass spectrometry (ICP-MS)² for kimchi origin classification. ICP-MS achieved the highest accuracy (100%) but requires complex sample preparation and expensive equipment. ICP-OES offered a strong balance with 98% accuracy and moderate complexity. LIBS, requiring minimal sample preparation and offering lower operational costs, achieved 92.8% accuracy, making it suitable for rapid screening. Ultimately, method selection should be guided by the specific requirements for precision, speed, and practicality.

Keywords: Kimchi, ICP-OES, Machine learning, Elemental analysis, Food authentication



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ESTIMATION OF TOTAL PHENOLIC CONTENT AND TOTAL CARBONYL COMPOUNDS FOR IDENTIFYING NATURAL RUBBER SHEET SMUGGLING INTO THAILAND

Orapan Apirakkan^{a,*}, Neungrutai Saesaengseerung^a, Orasa Onjun^a

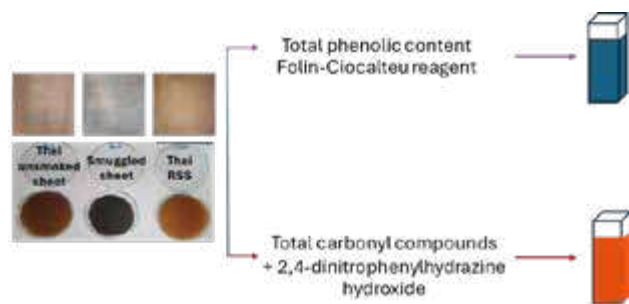
^aDepartment of Science Service (DSS), 75/7 Rama VI Road, Ratchathewi Bangkok 10400, Thailand

*Corresponding author: aorapan@dss.go.th

Abstract

Thailand is a leading natural rubber producer and exporter. However, fluctuations in rubber prices, particularly the sharp increase in 2024, have led to the smuggling of rubber sheets from foreign countries. To protect Thai rubber producers and economy, it is crucial to distinguish Thai ribbed smoked sheets (RSS) from smuggled rubber sheets. This study aims to identify smuggled rubber sheets through visual and chemical analysis. Three types of rubber—Thai unsmoked rubber sheets, smuggled rubber sheets, and Thai ribbed smoked sheets (RSS)—were examined. Visually, smuggled rubber sheets differ in color, cleanliness, and blemishes. By Chemical analysis, total phenolic content (TPC) and total carbonyl compounds (TCC) were measured to differentiate these rubber sheets. Circular rubber specimens (9 cm in diameter) were soaked in 25 mL of methanol for 120 minutes to extract phenolic and carbonyl compounds from the surface. TPC and TCC in the extract were analyzed using a spectrophotometer, each with a different reagent and absorbance wavelength. TPC was determined using the Folin-Ciocalteu reagent, with gallic acid as the standard, and its absorbance was measured at 765 nm. In contrast, TCC was quantified by reacting the extract with an acidic 2,4-dinitrophenylhydrazine hydroxide solution, using 2-butanone as the standard, with detection at 480 nm [1]. The results demonstrated that Thai RSS exhibited the highest TPC value ($4.5 \mu\text{g GAE}/\text{cm}^2$), approximately three times greater than that of Thai unsmoked sheets and smuggled rubber sheets. However, smuggled rubber sheets contained the highest TCC level ($0.005 \mu\text{g CO}/\text{cm}^2$), followed by Thai RSS ($0.002 \mu\text{g CO}/\text{cm}^2$) and Thai unsmoked sheets ($0.001 \mu\text{g CO}/\text{cm}^2$). The high TPC value in Thai RSS is attributed to the smoking process, whereas the relatively low TPC in smuggled rubber sheets suggest suboptimal smoking conditions, such as lower temperatures or incomplete processing. The TCC findings align with the observable characteristics of smuggled rubber sheets, which emit a stronger, unpleasant odor compared to other samples. These findings indicate that TPC and TCC measurements can effectively distinguish smuggled rubber sheets, providing a reliable analytical approach for identifying smuggled rubber products.

Keywords: Ribbed smoked sheets (RSS), Total phenolic contents, Total carbonyl compounds



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ADVANCING BIODEGRADABLE POLYMER FIBER PRODUCTION WITH MELT ELECTROSPINNING

Yejin Lee^a, Yun Hyeong Lee^a, Byung-Kwon Kim^{a*}

^aEwha Womans University

*Corresponding author: kimb@ewha.ac.kr

Abstract

Biodegradable polymers (BPs) are widely used in various fields, including textile fibers and biomedical applications. [1] In this context, the melt electrospinning (MES) technique, which is solvent-free and involves both thermal processing and electrostatic force during production, provides a versatile method for fabricating fibers from BPs. [2] Controlling the conductivity and viscosity of BP solutions plays a pivotal role in MES, enabling the production of thin fibers with a high surface-area-to-volume ratio. [3] However, polymer solutions generally have low conductivity and high viscosity, making the production of microfibers or nanofibers challenging. To address this issue, previous studies have introduced polyphenol-based additives. [4] Electrochemical and rheological analyses of BP solutions were conducted to identify the effective types and concentrations of additives. Based on these results, MES was successfully employed to fabricate nanofibers, and their structural and chemical properties were subsequently evaluated. A further experiment involving cell co-seeding was conducted to assess the biological response of the electrospun fibers. These findings offer information on the potential uses of modified polymer fibers in biomedical fields.

Keywords: biodegradable polymer, melt electrospinning, electrochemistry, biocompatibility

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COMPARISON OF HCl: HNO₃ COMPOSITION IN THE DESTRUCTION OF Pb AND Cu IN THE SURFACE SEDIMENT OF THE MANGROVE FOREST OF THE MUARA NUSA DUA RESERVOIR

Irdhawati^{a*}, I Nengah Simpen^b, Maria Goreti Ling^a

^aAnalytical Chemistry Division, Department of Chemistry, Faculty of Science, Udayana University, 80361 Indonesia

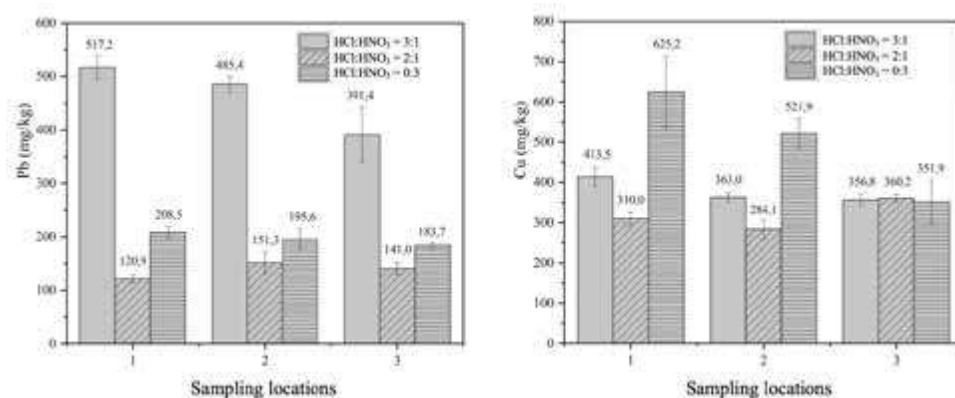
^bPhysical Chemistry Division, Department of Chemistry, Faculty of Science, Udayana University, 80361 Indonesia

*Corresponding author: irdhawati@unud.ac.id

Abstract

The Muara Nusa Dua Reservoir area is a reservoir that serves as a source of raw water in south Bali. This study aims to determine the composition of HNO₃ and HCl solvents on the destruction ability of Pb and Cu in the Muara Nusa Dua Reservoir Surface sediment. Metal dissolution in sediment was carried out using the wet destruction method; then the metal concentration was analyzed using an Atomic Absorption Spectrophotometer (AAS). The results showed that the total concentration of Pb and Cu in three locations, the highest, was found at location 1, namely Pb with a solvent composition of HCl and HNO₃=2:1 for Pb and Cu=2:1 at locations 2 and 3. The total concentration of Pb and Cu with a composition solvent of 3:1 in the sediment ranged from 391.4 ± 50.3 ~ 517.5 ± 22.5 mg/kg and 356.8 ± 14.8 ~ 413.5 ± 23.6 mg/kg. In the composition solvent of 2:1, the total concentration of Pb and Cu ranged from 120.9 ± 7.6 ~ 151.3 ± 20.6 mg/kg and 284.1 ± 23.0 ~ 360.2 ± 9.6 mg/kg. For Pb and Cu, the composition solvent of 0:3 ranged from 183.7 ± 4.8 ~ 208.5 ± 10.4 mg/kg and 351.9 ± 54.6 ~ 625.2 ± 88.8 mg/kg. The concentration of Pb and Cu has exceeded the standard quality threshold for Pb and Cu according to ANZECC (2000) of 50 mg/kg and 65 mg/kg. Based on the analysis results, it can be concluded that the best solvent composition for the destruction of Pb and Cu in the surface sediment of the Mangrove Forest in the Muara Nusa Dua Reservoir, obtained at a composition of 3:1 for Pb and 0:3 for Cu.

Keywords: wet destruction, HCl, HNO₃, heavy metals, surface sediment



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ANALYTICAL EVALUATION OF ANTIMICROBIAL PROPERTIES OF PARAPROBIOTIC *LACTOBACILLUS RHAMNOSUS* FOR COSMECEUTICAL APPLICATIONS

Pervin Soyer^a, A. Alper Öztürk^{b*}

^aAnadolu University, Faculty of Pharmacy, Department of Pharmaceutical Microbiology, Eskisehir, Türkiye.

^bAnadolu University, Faculty of Pharmacy, Department of Pharmaceutical Technology, Eskisehir, Türkiye.

*Corresponding author: aaozturk@anadolu.edu.tr

Abstract

In recent years, the use of probiotics and paraprobiotics in skin care formulations has gained increasing interest due to their potential to improve skin barrier integrity, modulate immune responses, and maintain microbial balance. *Lactobacillus rhamnosus* GG (LGG), a well-characterized probiotic strain, exhibits notable anti-inflammatory and antioxidant properties that may benefit individuals with skin conditions such as eczema, atopic dermatitis, and acne vulgaris. Unlike live probiotics, paraprobiotics-defined as non-viable microbial cells or cell components that confer health benefits-offer improved safety, stability, and compatibility for topical applications. However, analytical validation of their bioactivity remains essential for regulatory and formulation purposes. This study aimed to evaluate the antimicrobial potential of sonication-inactivated LGG using standard microbiological assays.¹ LGG bacterial cells were inactivated using probe sonication, a method shown to preserve functional cell wall components responsible for immunomodulatory and antimicrobial effects. The resulting paraprobiotic suspension was tested for antimicrobial activity using disc diffusion and microdilution techniques in accordance with CLSI (*Clinical and Laboratory Standards Institute*) guidelines. A panel of microbial strains was used, including *Pseudomonas aeruginosa* ATCC 27853, *Staphylococcus aureus* ATCC 29213, *Bacillus subtilis* NRRL B478, *Escherichia coli* ATCC 35218, *Candida albicans* ATCC 90028, and *Candida krusei* ATCC 6258.²⁻⁴ The LGG-derived paraprobiotic exhibited dose-dependent antimicrobial activity. At 18 mg.mL⁻¹, inhibition zones were observed against Gram-positive and Gram-negative bacteria, while antifungal activity against *Candida* spp. was recorded at 9 mg.mL⁻¹. These findings indicate the preserved antimicrobial potential of LGG even after inactivation. The reproducibility and clarity of the inhibition zones confirmed the efficacy of the method used and highlighted the paraprobiotic's analytical detectability. Paraprobiotic LGG demonstrated measurable antimicrobial activity, supporting its suitability for cosmeceutical product development. These results suggest that inactivated probiotic components could serve as bioactive ingredients in topical pharmaceutical and skin care formulations. Further studies will focus on complementary biological activities such as antibiofilm, antioxidant, and cytotoxic effects to explore broader dermatological applications.

Keywords: *Lactobacillus rhamnosus*, Paraprobiotic, Antimicrobial activity, Analytical evaluation, Cosmeceuticals, Skin health

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GEOGRAPHICAL VARIATION IN PHYTOCHEMICAL COMPOSITION OF *EURYCOMA LONGIFOLIA* ROOT EXTRACTS AND THEIR ANTI-SARS-COV-2 ACTIVITY

Norazlan Mohmad Misnan^{a,b*}, Lam Kok Wai^b, Maizatul Hasyima Omar^a,
Mohd Ridzuan Mohd Abd Razak^a

^aHerbal Medicine Research Centre, Institute for Medical Research, National Institutes of Health, Ministry of Health Malaysia, Shah Alam 40170, Selangor, Malaysia

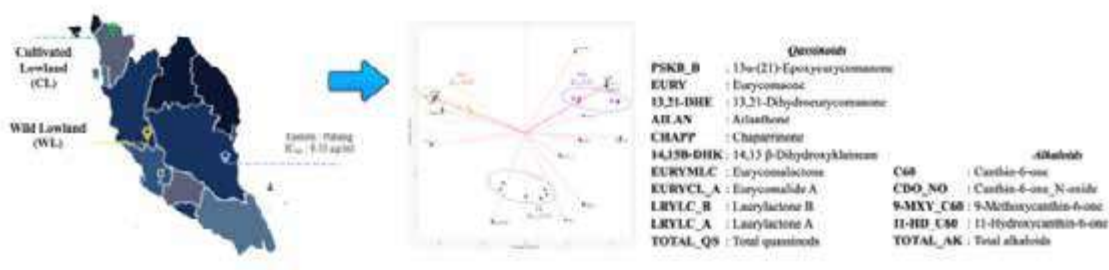
^bCentre for Drug and Herbal Development, Faculty of Pharmacy, Universiti Kebangsaan Malaysia, Jalan Raja Muda Abdul Aziz, Kuala Lumpur 50300, Malaysia

*Corresponding author: norazlan.misnan@moh.gov.my

Abstract

Eurycoma longifolia, commonly known as Tongkat Ali is a well-known medicinal plant found throughout Malaysia. The content of bioactive compounds in the root extracts which have potential in combating viral infections may vary depending on geographical location and environmental conditions. This study aimed to investigate the anti-SARS-CoV-2 activity of *E. longifolia* root extracts from different geographical locations in Malaysia and to correlate the activity with their phytochemical composition. *E. longifolia* roots were collected from three sampling sites in Peninsular Malaysia: wild highland (WH), cultivated lowland (CL), and wild lowland (WL). Root extracts were screened for anti-SARS-CoV-2 activity in vitro using Vero E6 cells. Fourteen known compounds including quassinoids and alkaloids, were quantified using LC-MS. Multivariate analysis was used to establish correlations between phytochemical composition and antiviral activity. *E. longifolia* root extracts from WH showed the highest anti-SARS-CoV-2 activity (IC₅₀ 9.33 µg/ml), followed by WL (IC₅₀ 13.31 µg/ml) and CL (IC₅₀ 18.47 µg/ml) samples. Multivariate analysis revealed that quassinoid compounds were strongly associated with the samples showing the highest antiviral activity. Alkaloids were predominantly found in CL samples, which showed the lowest anti-SARS-CoV-2 activity. The variation in antiviral activity due to different geographical locations highlights the importance of considering the source of the plant when evaluating its therapeutic potential. The strong correlation between quassinoid content and antiviral activity suggests that these compounds may be responsible for the observed effects. The negative association between alkaloid content and antiviral activity in CL samples suggests possible antagonistic effects, which require further investigation. This study gives useful information about how the anti-SARS-CoV-2 activity of *E. longifolia* varies by location. It also shows how this activity is linked to the plant's chemical content, which can help guide future studies and possible treatment development for COVID-19.

Keywords: *Eurycoma longifolia*, Phytochemicals, COVID-19, Quassinoids, Geographical variability



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EXAMINATION OF PHOTODYNAMIC THERAPY BY AMBIENT MASS SPECTROMETRY

Yiyan Yin^a, Jin Ouyang^{a,b}, Na Na^{a*}

^aKey Laboratory of Radiopharmaceuticals, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing, 100875, China.

^bDepartment of Chemistry, Faculty of Arts and Sciences, Beijing Normal University, Zhuhai, 519085, China.

*Corresponding author: nana@bnu.edu.cn

Abstract

Photodynamic therapy (PDT) has exhibited great potential in tumor therapy due to its significant advantages of spatiotemporal selectivity and low biological toxicity. Considering the process of PDT involving series of molecular structural changes, the monitoring and examinations of these biological changes in the biological environment are crucial for improving and developing the efficient therapy strategies. However, the monitoring of biomolecules is normally challenged by various interferences from the complex biological environment. Moreover, multiple side reactions in PDT are even significant challenges for the examination of therapy processes. Recently, *in situ* synthesis of drugs in tumors has obtained great interests due to its advantages of achieving precise tumor treatment and avoiding side effects on normal tissues. Therefore, it is of great significance to monitor the metabolic process and structural changes during PDT upon the *in situ* synthesis of therapy reagents. Ambient mass spectrometry (AMS) enables direct capture and identification of intermediates in the reaction systems without or with less pretreatment, holding significant advantages in investigating reaction mechanisms in complex systems.¹ Various AMS methods have been systematically developed for monitoring and investigation of diverse reactions, including enzyme-catalyzed reactions, and some biochemical processes during a certain therapy.²⁻⁴ Consequently, AMS will demonstrate unique advantages in monitoring of multiple molecules during the process of tumor treatments. Herein, the *in-situ* synthesis of a 2D/2D C₃N₄-MnO₂ single-atom catalysts (C₃N₄-Mn SACs) was reported for the tumor-selective PDT cancer treatments,⁵ which was further monitored by AMS for mechanism examinations. In the tumor microenvironment, MnO₂ is reduced to Mn²⁺ by the upregulated GSH and subsequently coordinate with C₃N₄. This enabled the *in situ* synthesis of C₃N₄-Mn SACs in the tumor sites. Thereafter, hydroxyl radicals were generated under irradiation, which facilitated the PDT process to kill cancer cells. Upon the AMS monitoring and other comprehensive characterizations, the consumption of GSH and the mechanism of water splitting to produce hydroxyl radicals was demonstrated. Meanwhile, the hydroxyl radical induced lipid peroxidation was confirmed by detecting and analyzing lipids. As resulted, the important intermediates with cytotoxicity were observed by AMS during the fragmentation of lipid peroxides, which cleared the therapy mechanism of the present strategy. This work not only expands the application of AMS into the monitoring and mechanism examination of PDT process, but also provides a sufficient theoretical support for the development of new therapy strategies.

Keywords: Ambient mass spectrometry, Monitoring, Mechanism study, photodynamic therapy, lipid peroxidation.

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AUTOMATED SAMPLE PREPARATION OF OPIOIDS IN BLOOD AND URINE SAMPLES FOR THE DETERMINATION BY LIQUID CHROMATOGRAPHY TANDEM-MASS SPECTROMETRY (LC-MS/MS)

Sharmilah Kuppusami^{a*}, Zul Helmi Salleh^a, Nor Azmi Abd Karim^a

^a*Toxicology Division, Forensic Analysis Science Centre, Department of Chemistry Malaysia, Petaling Jaya.*

**Corresponding author: sharmilah@kimia.gov.my*

Abstract

Liquid chromatography-tandem mass spectrometry (LC-MS/MS) is a highly effective technique for the routine quantification of drugs of abuse in biological matrices such as blood and urine. However, traditional manual sample preparation methods are often time-consuming and can introduce variability. To address this, the Toxicology Division of the Forensic Science Analysis Centre, Department of Chemistry Malaysia, has developed an automated sample preparation protocol utilizing the Tecan Freedom EVO liquid handling system for the quantification of opioids in whole blood and urine by LC-MS/MS. The automated process includes spiking with calibration standards, addition of internal standards, and protein precipitation via organic solvent addition. Following centrifugation, the pre-treated samples undergo solid-phase extraction using cartridges before LC-MS/MS analysis. Manual intervention is limited to transferring sample tubes between the robotic system and the centrifuge, and transferring eluted samples to the LC autosampler. This study focused on five opioids: hydromorphone, hydrocodone, morphine, codeine, and 6-monoacetylmorphine. Method validation parameters, including linearity, precision, accuracy, limit of detection (LOD), and limit of quantitation (LOQ), were determined. Results obtained from automated sample preparation demonstrated close agreement with those from manual methods. In conclusion, the described analytical system, which integrates automated solid-phase extraction with LC-MS/MS analysis, offers a convenient, precise, and accurate approach. It significantly reduces hands-on time, solvent exposure, and potential human error, while also improving the efficiency of LC-MS/MS data integration by providing consistent results.

Keywords: automation, opioids, solid-phase extraction, blood, urine

AUTOMATED NMR ACQUISITION AND PROCESSING FOR HIGH-THROUGHPUT ANALYTICAL QUALITY MANAGEMENT

Sean Bowen^{a*}

^a*Incyte Corporation*

**Corresponding author: sbowen@incyte.com*

Abstract

Routine NMR analysis often serves as a bottleneck in high-throughput workflows, particularly when sample preparation, parameter adjustment, and data processing require manual input. Not only is this input time-consuming, but it also introduces variability. We have implemented a fully automated workflow that processes all submitted compounds without intervention, ensuring consistency and reproducibility across a large and chemically diverse sample set. To build a robust and fully automated pipeline for 1D NMR acquisition and processing that ensures reproducible results, minimizes user burden, and generates structured, traceable datasets suitable for both routine analysis and long-term reuse. Samples are prepared from weekly plates of DMSO stocks, with no manual handling or preparation. Each sample is initially scanned in a short scout experiment (<2 s) to identify solvent peaks. Suppression is then automatically tailored to each sample based on these results, without requiring predefined solvent information. The main acquisition proceeds using standard parameters. Spectra are processed automatically with baseline correction, multiplet-aware filtering, and exclusion of common artifacts such as ammonium triplets. Signal-to-noise ratios, integral-per-proton values, and impurity ratios are calculated automatically. Structured outputs are generated in machine-readable formats. Sample-level metadata, including solvent, pulse program, and quality metrics are recorded in a lightweight SQL-based system. This provides many of the advantages of a LIMS, such as traceability and structured reporting, without the complexity or overhead. The system processes over 20,000 compounds per year. All data are archived in a searchable format that supports batch comparison, structure verification, and publication. The workflow is fully unattended and reproducible across large datasets. This platform enables scalable, hands-free NMR analysis and creates a high-quality spectral dataset suitable for downstream applications including machine learning and automated quality assessment.

Keywords: NMR automation, solvent suppression, reproducibility, metadata, high-throughput analysis, chemometrics

I-SPECTROCHEM CHEMOMETRICS MULTIVARIATE: RAPID DETERMINATION OF KINEMATIC VISCOSITY (KV) & SIMDIST HIGH TEMPERATURE (HT) IN VACUUM GASOIL

Wan Ahmad Rosidi Bin Wan Derahman; Muhamad Zaki Bin Ibrahim; Mohd Izzat Bin Sulaiman

Malaysian Refining Company Sdn Bhd. (MRCSB)

**Corresponding author: wrosidi_wderahman@petronas.com; zaki.ibrahim@petronas.com.my;*

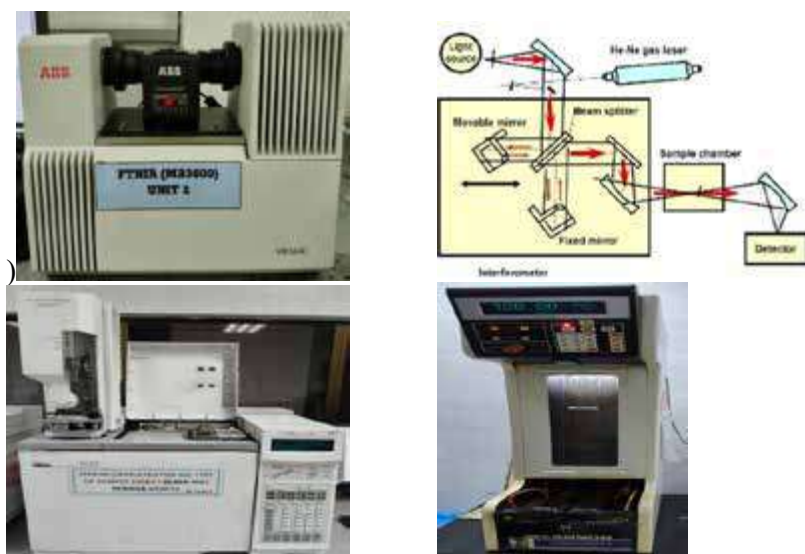
izzat_sulaiman@petronas.com.my

Abstract

The kinematic viscosity of various petroleum fuels, utilized as lubricants, is crucial for determining optimal storage, handling, and operational conditions. The boiling range distribution of medium and heavy petroleum distillate fractions offers insights into the composition of feedstocks and products associated with petroleum refining processes, such as hydrocracking, hydrotreating, visbreaking, and deasphalting. This test method can be employed for product specification testing upon mutual agreement of the involved parties. Instead of traditional methods, kinematic viscosity and high-temperature simulation distillation testing will utilize a universal heated vial in conjunction with Fourier Transform Near Infrared (FT-NIR) spectroscopy, coupled with chemometric and multivariate analysis techniques. This approach leverages chemical characteristics and statistical data analysis for enhanced accuracy.

Keywords: FTNIR, Chemometric Multivariate, Distillation, Kinematic Viscosity, Universal Heated Vial.

Graphic / Image



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IMPROVED EFFICIENCY AND TIME CONSUMPTION FOR LEAD ANALYSIS IN GASOLINE BY XRF

M Hafiz bin Azman, M Zaki Ibrahim, M Izzat Sulaiman

Malaysian Refining Company Sdn. Bhd.

*Corresponding author: hafiz_azman@petronas.com

Abstract

New standard method for MRCSB with compliance to ASTM D5059 has been successfully developed by MRCSB lab. ASTM D5059 determines Lead (Pb) in Gasoline by X-Ray Fluorescence Spectroscopy (EDRFX). Analysis of live sample by ASTM D5059C gives consistent reading below calibration point <0.0013 g/L as compact to current conventional method by IP224. Although IP 224 can measure as low as 3 ppb, this method quite lengthy and time consumption as compared to XRF method, therefore ASTM D5059C is acceptable for ULG product certification.

Analysis by ASTM D5059C is **more effective** with high accuracy and precision. Advantages are as follows.

- faster analysis time (3 min)
- minimal sample pretreatment and no digestion
- multiple samples determination in one analysis sequence
- less chemical exposure

MRCSB lab has demonstrated following capabilities from the method development:

- **excellent accuracy** of 102.6% (tolerance 80-110%)
- **better site precision** of 0.0013 g/L against method precision 0.0048 g/L
- highly **sensitive detection** with lowest limit at 0.0013 g/L, below ASTM range of 0.0026 kg/L
- **consistent measurement** of MRCSB live Gasoline samples at <0.0013 g/

As a result, ASTM D5059C is acceptable for certification of unleaded gasoline products due to its consistency and sensitivity.

Keywords: Lead (Pb) in Gasoline, Gasoline by X-Ray Fluorescence Spectroscopy (EDRFX), ASTM D5059C

Comparison of Live Sample using ASTM D5059C versus IP224

No	Date	Tank	ASTM D5059		IP 224, g/L	Product Spec, g/L
			Actual Result, g/L	Report as per method, g/L		
1	25-Jul-24	7508	-0.0016	<0.0026	<0.000003	<0.013
2	27-Jul-24	7506	-0.0013	<0.0026	<0.000003	<0.013
3	26-Jul-24	7506	0.0004	<0.0026	<0.000003	<0.013
4	24-Jul-24	7503	-0.0012	<0.0026	<0.000003	<0.013
5	12-Jul-24	7503	-0.0014	<0.0026	<0.000003	<0.013
6	12-Jul-24	7507	0.0003	<0.0026	<0.000003	<0.013
7	13-Jul-24	7507	-0.0013	<0.0026	<0.000003	<0.013
8	6-Jul-24	7508	-0.0008	<0.0026	<0.000003	<0.013
9	30-Jun-24	7504	-0.0012	<0.0026	<0.000003	<0.013
10	25-Jul-24	7508	-0.0013	<0.0026	<0.000003	<0.013
11	27-Jul-24	7506	-0.0007	<0.0026	<0.000003	<0.013
12	26-Jul-24	7506	-0.0010	<0.0026	<0.000003	<0.013
13	24-Jul-24	7508	-0.0011	<0.0026	<0.000003	<0.013
14	12-Jul-24	7503	-0.0014	<0.0026	<0.000003	<0.013
15	12-Jul-24	7507	-0.0010	<0.0026	<0.000003	<0.013
16	13-Jul-24	7507	-0.0010	<0.0026	<0.000003	<0.013

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EFFECT OF PH ON THE FORMATION OF CYANIDE ION-CURCUMIN COLOUR COMPLEXES FOR DETECTION OF CYPERMETHRIN IN TREATED WOOD

Tumirah Khadiran^{a*}, Nuraqilah Mardhiah Samsul Alam^b, Mohd Amirul Mukmin Abdullah^a

^a*Wood Protection Branch, Forest Products Division, Forest Research Institute Malaysia (FRIM),
52109 Kepong Selangor*

^b*School of Chemical Engineering, University Technology Mara (UiTM), Bukit Besi, Terengganu*

**Corresponding author: tumirah@frim.gov.my*

Abstract

Cypermethrin has been widely used as an effective wood preservative to protect timber against insect attacks, particularly termites and wood-boring beetles, by acting as a long-lasting synthetic pyrethroid insecticide. The colorimetric assay technique is one of the simplest and most cost-effective methods to measure cypermethrin in treated wood samples by converting it into cyanide ions through a hydrolysis process, which then reacts with curcumin reagent to form a color complex^{1,2}. The aim of this study is to analyze the effect of pH on color complex formation, as it can influence the stability, intensity, and formation rate of the complex, potentially affecting the sensitivity and accuracy of colorimetric assays. To check the effect of different pH condition on the formation of colour complex, the absorption band at wavelength of 200-1000 nm were examined. The findings suggesting that cyanide ion-curcumin complexes does not exist at acidic pH. However, at basic pH of 10.5, the adsorption band at 520 nm heightened rapidly and the colour of the solution to reddish orange³. The results showed that curcumin is a sensitive colour reagent with respect to pH and could be applied as a colorimetric assay method for the determination of cypermethrin in treated wood.

Keyword: Cypermethrin, cyanide ion, curcumin, treated wood, colorimetric assay

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ELECTROCHEMICAL DETECTION OF OXYBENZONE USING POLYPYRROLE-IMPRINTED POLYMER MODIFIED SCREEN-PRINTED GOLD ELECTRODE

**Mohd Azerulazree Jamilan^{a,*}, Vinotdhni Kanthymathynathan^b, Mohd Fairulnizal Md Noh^a,
Faizatul Shimal Mehamod^{b,c}**

^a *Nutrition Unit, Nutrition, Metabolism and Cardiovascular Research Centre*

Institute for Medical Research, National Institute of Health, Ministry of Health Malaysia

Malaysia, No. 1, Jalan Setia Murni U13/52, Setia Alam, 40170 Shah Alam, Selangor D.E., Malaysia.

^b *Faculty of Science and Environmental Marine, Universiti Malaysia Terengganu, 21030, Kuala Nerus, Terengganu, Malaysia.*

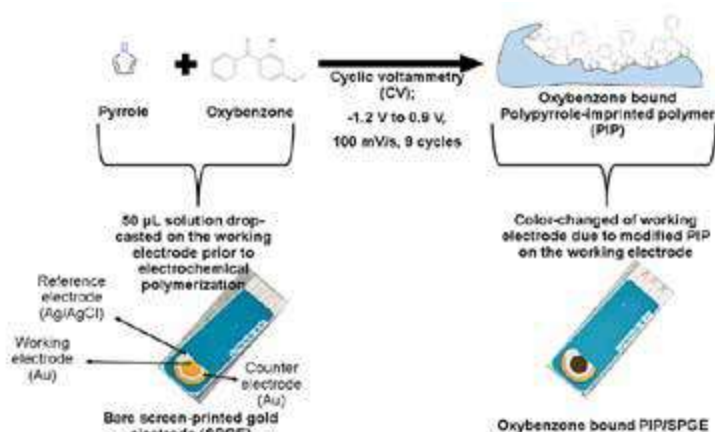
^c *Advanced Nano Materials (ANoMA) Research Group, Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030, Kuala Nerus, Terengganu, Malaysia*

^{*}Corresponding author: azerulazree@moh.gov.my

Abstract

Oxybenzone (or benzophenone-3) is a widely used chemical for sunscreen products for absorbing ultraviolet (UV) radiation to protect the human skin from sunburn, premature aging and skin cancer. Nevertheless, its environmental effect caused oxybenzone to be found in various fish species, posing risks to marine ecosystems and coral reef bleaching. The detection of a more portable and easy-to-use approach was deemed necessary to monitor the levels of oxybenzone as some areas, such as Hawaii, United States of America (USA), banned the use of oxybenzone in sunscreens. Here, we developed an electrochemical polymerized polypyrrole-imprinted polymer on the screen-printed gold electrode (PIP/SPCE) specific for oxybenzone detection. The electrochemical polymerization was optimized by the cyclic voltammetry (CV) scan cycle number (9 cycles), the template leaching solution (0.1 M hydrochloric acid, HCl), and template-monomer molar ratio (1:15). The modified PIP/SPCE was characterized with electrochemical impedance spectroscopy (EIS), Fourier-transform infrared (FTIR) spectroscopy, and field emission scanning electron microscopy (FESEM) confirmed the presence of electrochemical polymerized PIP on the SPGE. The calibration was found to be linear ($R^2=0.9814$; $y=0.166x+1.0726$) from 5.0 μM to 40.0 μM , with a detection limit of 14.4 μM . Spiked water samples resulted in excellent recovery from 85% to 87%. The modified PIP/SPCE proved to be a practical alternative method for the detection of oxybenzone in water samples.

Keywords: eMIP, screen-printed electrode, electrochemical polymerization, electrochemical detection, water sample



IN-SYRINGE DISPERSIVE MICRO SOLID PHASE EXTRACTION METHOD FOR AFLATOXINS IN PEANUT BY HPLC

Nor Shifa Shuib^{a,*}, Bahrudin Saad^b

^a*Environmental and Industry Analysis, Department of Chemistry Malaysia, George Town, Pulau Pinang, Malaysia.*

^b*School of Chemical Science, Universiti Sains Malaysia, George Town, Pulau Pinang, Malaysia.*

*Corresponding author: norshifa@kimia.gov.my

Abstract

The simultaneous determination of aflatoxins (B_1 , B_2 , G_1 and G_2) in peanut using in-syringe dispersive micro-solid phase extraction (ISD μ SPE) coupled with high performance liquid chromatography with fluorescence detection is described. The samples (25g) were extracted after mixed with 125 ml methanol:water (6:4, v/v) and 5 g of sodium chloride. Then the extracts were filtered with Whatman filter paper (No. 4). The filtrate (20 ml) were diluted to 50 ml with water. The diluted filtrate (2.5 ml) was mixed with dispersive sorbent in a syringe that was attached with glass fiber syringe filter (25 mm I.D and 0.7 μ m pore size). Samples were vortexed and passed through the glass fiber syringe filter followed by washing, elution and evaporation processes. Then, the residue was reconstituted in 200 μ L of methanol and water (1:1, (v/v)) for HPLC determination. The separation of aflatoxins was performed using C18 Hypersil gold (250 mm x 4.6 mm, 5 μ m) column at 40°C. The excitation and emission wavelength of the fluorescence detector was set at 360 nm and 440 nm, respectively. On-line photo-chemical derivatisation was used to enhance the detection of aflatoxin B_1 and G_1 . Limits of quantification (LOQ) ranged from 0.66 to 0.90 μ g kg⁻¹, recoveries from 77.8 to 114.7 % and relative standard deviations (RSD) from 2.0 to 12.3%.

Keywords: Aflatoxins, syringe, HPLC

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QUANTIFICATION OF CAFFEINE AND TRIGONELLINE IN MALAYSIAN INSTANT COFFEE PRODUCTS USING VALIDATED RP-HPLC METHOD

Yen Mae Lee^a, Cherlyn Cheng Chen Xi^a and Lai Chun Wong^{a*}

^aIMU University

*Corresponding author: laichunwong@imu.edu.my

Abstract

Caffeine and trigonelline are key bioactive alkaloids present in coffee, influencing both its sensory properties and physiological effects ^{1,2}. While moderate consumption is associated with potential health benefits, excessive intake, especially caffeine, can pose health risks ³. This study presents a validated reverse-phase high-performance liquid chromatography (RP-HPLC) method for the simultaneous determination of caffeine and trigonelline in commercially available instant coffee samples in Malaysia.

Chromatographic separation was achieved using a GraceSmart RP C18 column with gradient elution of methanol and water. The method demonstrated good linearity, precision, and recovery, in accordance with validation requirements for quantitative analysis. Fifteen instant coffee products were analysed, revealing a wide variation in alkaloid content. The caffeine content of several products approached levels that could contribute significantly to the daily maximum intake recommended by regulatory agencies. These findings highlight the need for stringent quality control and transparent labelling in the coffee industry. The validated method offers a reliable approach for routine monitoring of coffee alkaloids, supporting consumer awareness and regulatory compliance.

Keywords: caffeine, trigonelline, instant coffee, reverse-phase high-performance liquid chromatography, validation

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COLORIMETRIC METHODS AS GREEN ANALYTICAL CHEMISTRY TOOLS IN FUEL AND BIOFUEL QUALITY CONTROL

**Paola A. Mello^{a,*}, Alice P. Holkem^a, Gabrielle D. Iop^a, Flavia F. Oliveira^a,
Rochele S. Picoloto^a, Juliano S. Barin^b, Edson I. Müller^a**

^a Departamento de Química, ^b Departamento de Ciência e Tecnologia dos Alimentos, Universidade Federal de Santa Maria (UFSM), Santa Maria 97105-900, Brazil

*Corresponding author: paola.mello@ufsm.br

Abstract

The development of digital image-based methods (DIB) stands out among the advances in alternative methods for chemical analysis. Obtaining and processing images related to processes or reaction are viable alternatives in various chemical analyses due to the lower cost and acquisition time, combining a potential for *in situ* operation, feasibility of real-time analysis and automation.¹ In addition, the ease of use, versatility and the possibility of being a non-invasive and/or destructive method (in some cases) expand the scope of applications. However, the application of these systems to petroleum, fuels and biofuels has limitations and represents an analytical challenge. Among other factors, the solubility of reagents, the viscosity and the natural color of the samples, in comparison with other predominantly aqueous or water-soluble matrices, imply difficulties in the development of methods and compromise accuracy. Alternative methods based on DIB colorimetry have been developed for chloride in petroleum^{2,3} and ethanol⁴ and for determination of the basic nitrogen content in diesel oil⁵. For those developments, a portable device composed of a homemade 3D-printed chamber with a USB camera was used. The PhotoMetrix app was used and converted the images into RGB histograms, and a partial least squares (PLS) model was obtained from chemometric treatment, for each method. The PLS model was evaluated considering the coefficient of determination (R²) and the root mean square errors (RMSEs)—calibration (RMSEC), cross-validation (RMSECV), and prediction (RMSEP). Accuracy was evaluated by comparison with reference values, as follows: with ASTM D 6470 and direct solid sampling elemental analysis (for chloride in crude oil), with ASTM D 7328-23 (for chloride in ethanol fuel), and with UOP 269-10 (for basic nitrogen content in diesel oil). The easy-to-use colorimetric analysis offered high-throughput, low-cost, and environmentally friendly methods, with the possibility of portability. Additionally, the decrease in energy consumption and waste generation, increasing the sample throughput and operators' safety, makes the developed methods greener approaches. Furthermore, the cost savings make those methods suitable options for routine quality control, which can be attractive in the crude oil, fuels and biofuels industry.

Keywords: digital image-based methods, fuels, biofuels, crude oil, contaminants.

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RAPID IDENTIFICATION OF ANTIOXIDANTS IN BIODEGRADABLE PLASTICS BY SURFACE-ASSISTED LASER DESORPTION IONIZATION MASS SPECTROMETRY

Muyi He^a, Yun Ling^a, Chang Wang^a, Minli Yang^{a*}, Wei Guo^{a,*}

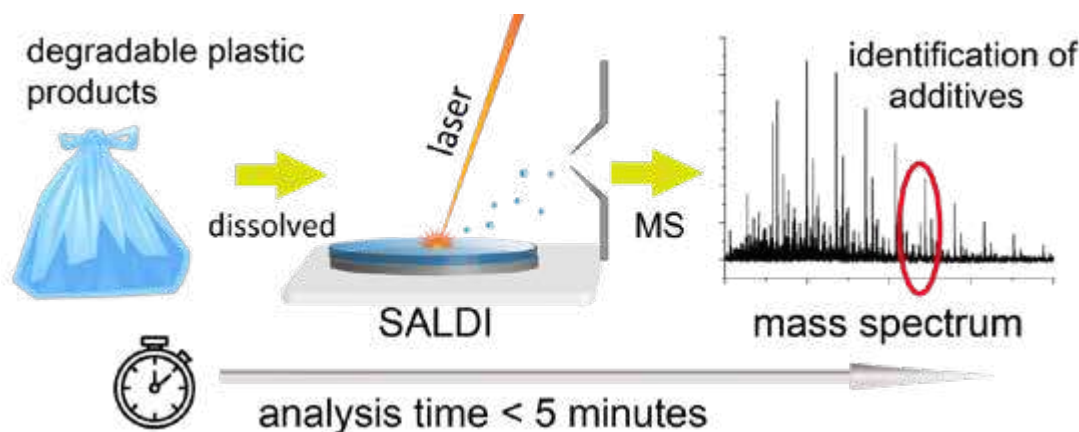
^a*Institute of Food Safety, Chinese Academy of Quality and Inspection & Testing*

**Corresponding author: 529513981@qq.com*

Abstract

The application of degradable plastics is of great significance to sustainable development. During the preparation of biodegradable plastics, antioxidants are added to prevent the polymer from degrading due to oxidation, thereby extending the life of the plastic and maintaining its physical properties. However, during the degradation process, additives may be released into the environment or food, posing risks of pollution and health hazards. In this study, a surface-assisted laser desorption/ionization mass spectrometry (SALDI-MS) method was developed for rapid identification and quantification of antioxidants in biodegradable plastics. Graphene oxide (GO) was utilized as an ionization assistant to enhance ionization efficiency and minimize background interference. The method was optimized using four common antioxidants (1098, 1520, 1726, and 3114), achieving reliable identification through accurate mass measurements and tandem MS analysis. Dynamic range curves were derived from standard solutions with determination coefficients exceeding 0.989. The performance of the method was also evaluated using authentic samples and commercially available biodegradable plastic products with recovery rates ranging from 78% to 109%, and limit of detection is 5.0 g/kg. Sample preparation is straightforward and the entire analytical process can be completed within just a few minutes. This method is suitable for rapid qualitative detection of additives in biodegradable plastics as well as quantitative evaluation of substance content variations during plastic degradation. It shows promise as a valuable tool for quality control and safety assurance in the plastic industry.

Keywords: biodegradable materials, polylactic acid, SALDI-MS, antioxidants rapid identification



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A COVALENT ORGANIC FRAMEWORK–COATED STEEL SUBSTRATE AS A MASS SPECTROMETRIC IONIZATION SOURCE FOR THE EFFECTIVE ENRICHMENT AND RAPID DETECTION OF PHTHALATES IN BEVERAGES

Minli Yang^a, Muiyi He^a, Yun Ling^a, Chang Wang^a

^aInstitute of Food Safety, Chinese Academy of Quality and Inspection & Testing

*Corresponding author: 529513981@qq.com

Abstract

A novel, rapid, and simple detection method is proposed to realize the simultaneous detection of seven phthalate esters (PAEs) within 1.5 min. A suitable covalent organic framework (COF) was coated on a stainless steel substrate (COFCS) to serve as both an enrichment element and a solid substrate for electrospray ionization mass spectrometry (ESI–MS). Twenty microliters of elution solvent was added dropwise to the COFCS enriched with analytes, and then high voltage electricity was applied and combined with ambient mass spectrometry (AMS) to realize the detection of PAEs. In order to investigate the reliability of the COFCS-ESI–MS method, dimethyl phthalate (DMP), diethyl phthalate (DEP), ethyl phthalate (2-methoxy) (DMEP), phthalate(2-ethoxy) ethyl ester (DEEP), dipentyl phthalate (DPP), dihexyl phthalate (DHXP), and butyl benzyl phthalate (BBP) were detected simultaneously. The proposed method showed good linearity in the range 0.1–80 µg/L with the determination coefficient (R^2) > 0.9916. The limits of detection (LODs) and limits of quantification (LOQs) of the determination technology were in the ranges 0.03–0.40 µg/L and 0.1–2.0 µg/L, respectively. The results demonstrated that the simultaneous detection of the seven PAEs in beverages can be realized using the method, and the spiked recoveries were in the range 85.17–104.09% with the relative standard deviations (RSDs) < 8.32%. In addition, the COFCS has good reusability and batch-to-batch repeatability and can be re-used at least 5 times and still maintain good enrichment performance.

Keywords Covalent organic frameworks · Ambient mass spectrometry · COFCS-ESI–MS · Phthalate esters



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MALAYSIAN COCOA VALIDATION PROGRAMME

**Badrul Hisyam Zainudin^{a,*}, Suzannah Sharif^a, Mohamed Yusof Ishak^b, Izzreen Ishak^a,
Chin Hui Han^a**

^a*Malaysian Cocoa Board, Cocoa Innovation and Technology Centre, Lot 12621 Kawasan Perindustrian Nilai, 71800 Nilai, Negeri Sembilan, Malaysia*

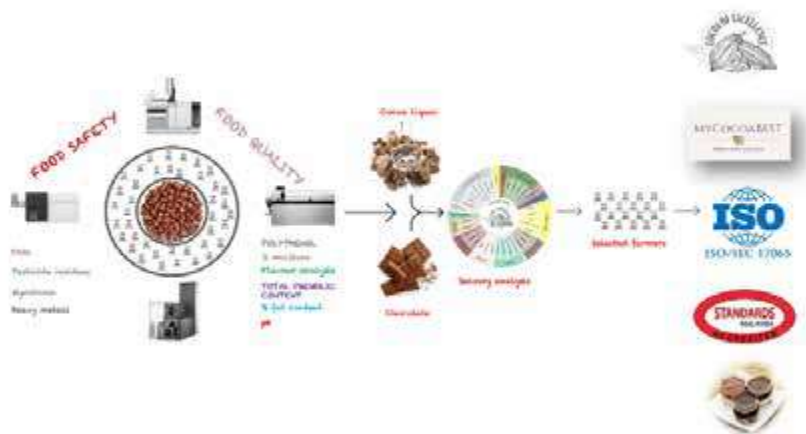
^b*Malaysian Cocoa Board, Trade Hub Facility Laboratory, Wisma PTP, Pelabuhan Tanjung Pelepas, Johor, Malaysia*

*Corresponding author: badrul@koko.gov.my

Abstract

The Malaysian Cocoa Validation Programme was conducted to evaluate the physical, chemical, and sensory properties of locally produced cocoa beans from 2022 to 2025. The screening process aimed to assess bean quality and identify potential improvements for cocoa bean trading and chocolate production. Physical properties were analyzed according to the Malaysian Standard MS 2672, ensuring compliance with industry benchmarks. Chemical analysis was divided into two categories: bean quality assessment, which examined parameters such as moisture content and fat composition, and food safety analysis^{1,2}, which included testing for contaminants and heavy metals and in accordance to the Malaysian Food Act 1985. Sensory evaluation was conducted following the Cacao of Excellence guidelines to determine the flavour profile and overall sensory characteristics of the beans. The findings revealed significant variation in the physical, chemical, and sensory attributes of Malaysian cocoa beans. Some beans demonstrated excellent quality, making them suitable for high-end chocolate production and export, while others exhibited deficiencies requiring corrective actions. The study provides a foundation for selecting the best beans for chocolatiers and traders, as well as identifying necessary interventions to improve bean quality. By addressing physical defects, optimizing chemical composition, and refining sensory characteristics, this programme aims to enhance the competitiveness of Malaysian cocoa in the global market. The results and corrective measures are further discussed in this study to support the continuous improvement of the Malaysian cocoa industry.

Keywords: Cocoa, food safety, food quality, sensory analysis



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DEVELOPMENT OF OPTICAL AND ELECTROCHEMICAL SENSORS AND BIOSENSORS UTILIZING BIS-NEOCUPROIN COPPER (II) COMPLEX (CUPRAC) AND ITS BIOTECHNOLOGICAL APPLICATIONS

Selen Ayaz ^{a*}, Yusuf Dilgin^a, Reşat Apak^b

^a Chemistry Department, Canakkale Onsekiz Mart University, Canakkale, Türkiye.

^b Chemistry Department, Istanbul University-Cerrahpasa, Istanbul, Türkiye.

*Corresponding author: selen.ayaz@comu.edu.tr

Abstract

The CUPRAC method is an electron transfer-based approach for assessing antioxidant capacity through the reduction of copper(II) ions. The approach was created by Dr. Reşat Apak and his colleagues in 2004¹. The work presents the development of two distinct research projects using sensors and biosensors one utilizing electrochemical methods and the other utilizing optical methods. Both studies are centered on the application of the copper(II) bis neocuproin complex (CUPRAC reagent). The first project involved adding the CUPRAC reagent to a glassy carbon electrode with multi-walled carbon nanotubes and analyzing the antioxidant capacity (21, various antioxidants) using an amperometric method with a flow injection analysis system. Cyclic voltammetric studies showed that the modified electrode exhibits a very well formed reversible redox couple for the Cu²⁺/Cu⁺ complex². The second part of the study used the CUPRAC reagent for three different substrate/enzyme groups: glucose, cholesterol, lactate, and pyruvate oxidase; glucose dehydrogenase; and acetylcholinesterase-AChE enzymes. Silanized magnetic nanoparticles were used to immobilize each enzyme. Optical enzymes based biosensors are presented that utilizes a colorimetric interaction between analytes and [Cu(Nc)₂]²⁺ complex. For this aim, the absorbance at 450 nm of the yellow-orange [Cu(Nc)₂]²⁺ formed through the colorimetric reaction of enzymatically produced analytes with [Cu(Nc)₂]²⁺ was recorded. An enzymatic reaction takes place on the NPs surface in the presence substrates. After the separation of NPs with a magnet, the enzymatically produced analytes chemically reduce the chromogenic oxidant cupric neocuproine to the cuprous chelate. The absorbances recorded for all analytes increased in direct proportion over a certain concentration range under optimized conditions. Fiber optic reflectometric biosensors were constructed utilizing hydrophilic polytetrafluoroethylene membranes, whereas fiber optic absorptimetric biosensors were developed employing a Nafion perfluorosulfonate-type membrane. Also, a pesticide biosensor was developed that employs the inhibition of AChE. The study concluded that three different analyte groups can be analyzed with the useful chromogenic oxidizing CUPRAC reagent, which is widely used in optical sensors: directly analyzing antioxidants and other reducing agents², indirectly analyzing non-reducing substrates^{3,4}, and indirectly analyzing pesticides that inhibit enzymes⁵.

Keywords: CUPRAC reagent, electrochemical sensor, magnetic nanoparticle, optical and fiber optic biosensor.

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EXPERIMENTAL DESIGN, AND ANALYTICAL PERFORMANCE OF ACTIVATED CARBON FOR MICROEXTRACTION OF POLYCYCLIC AROMATIC HYDROCARBONS IN *CAMELLIA SINENSIS*

Nur Zabirah Zabi¹, Wan Nazihah Wan Ibrahim^{1*}, Nordiana Suhada Mohmad Tahiruddin¹, Nurul Auni Zainal Abidin², Sazlinda Kamaruzaman³, Noorfatimah Yahaya⁴, Sheela Chandren⁵, Nursyamsyila Mat Hadzir¹

¹*Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia*

²*School of Chemistry and Environment, Faculty of Applied Sciences*

²*Universiti Teknologi MARA (UiTM), Cawangan Negeri Sembilan, Kampus Kuala Pilah, 72000 Kuala Pilah, Negeri Sembilan, Malaysia*

³*Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, Serdang, Selangor, Malaysia*

⁴*Integrative Medicine Cluster, Advanced Medical and Dental Institute (AMDI), Universiti Sains Malaysia, 13200 Bertam Kepala Batas, Penang, Malaysia*

⁵*Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia*

*Corresponding author e-mail: wannazihah@uitm.edu.my

Abstract

This research explores the development of circular economy green sorbents from agricultural waste for efficient sample pretreatment, focusing on activated carbon derived from empty fruit bunch fibres. The activated carbon was carbonised, encapsulated in alginate, and applied in dispersive solid-phase microextraction for the determination of four PAHs (naphthalene, fluorene, phenanthrene, and pyrene) in tea samples using HPLC–UV. The optimised Alg-ECB-AC beads/D- μ -SPE method demonstrated good linearity ($r^2 \geq 0.9909$), low detection limits (11–47 $\mu\text{g/L}$), and high relative recoveries (82.82%–118.22%). The innovative alginate encapsulation prevented self-agglomeration, enhancing sorption capacity. These findings highlight the potential of this sustainable sorbent for broader applications, including food safety monitoring.

QUANTIFICATION OF CHLORIDE INHIBITION OF OXYGEN REDUCTION IN BILIRUBIN OXIDASES USING PROTEIN FILM ELECTROCHEMISTRY

Amirah F. Kamaruddin^{a,b,c,*}, Nicolas Mano^{d,e}, Christopher F. Blanford^{a,b},

^aManchester Institute of Biotechnology, University of Manchester, 131 Princess Street, Manchester, M1 7DN, United Kingdom.

^bDepartment of Materials, University of Manchester, Oxford Road, Manchester, M1 3BB, United Kingdom.

^cDepartment of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 Skudai, Johor, Malaysia.

^dLe Centre National de la Recherche Scientifique (CNRS), CRPP, UPR 8641, F-33600 Pessac, France.

^eUniversité de Bordeaux, CRPP, UPR 8641, F- 33600 Pessac, France.

*Corresponding author: amirahfarhan@utm.my

Abstract

Bilirubin oxidases (BODs), a sub-group of multicopper oxidases (MCOs), have four Cu⁺/Cu²⁺ ions responsible for O₂ reduction coupled with the oxidation of bilirubin to biliverdin.¹ BODs display a high activity and stability at neutral pH, a high tolerance towards chloride anions and other chelators, and for some species, a high thermal tolerance.² They have gained more attention in numerous biotechnological applications under mild pH conditions, especially biofuel cells, bilirubin sensors, depollution, decolorization of dyes and pulp bleaching.^{1,2} The presence of halides in the environment inhibit the activity of MCOs and their halide tolerance varies enormously.³ In this present study, the inhibition modes of chlorides in BODs from fungus *Magnaporthe oryzae* (MoBOD) and bacterium *Bacillus pumilus* (BpBOD) were determined by quantitative measurements of O₂ inhibition obtained using protein film electrochemistry at pH 7 and at different temperatures (4°C, 25°C, 50°C and 60°C). The data from the electrochemical assays were fit to four inhibition models: competitive, uncompetitive, mixed and hyperbolic. Chlorides inhibition of O₂-reduction reaction catalysed by MoBOD and BpBOD were determined by the lowest reduced chi-squared values and an *F*-test analysis. Under continuous electrocatalysis, an electrode modified with BpBOD exhibits higher thermal stability and has a higher chloride tolerance than a MoBOD modified electrode, which is consistent with the literatures findings as bacterial MCOs generally have higher tolerance towards chlorides compared to fungal MCOs.^{4,5}

Keywords: Multicopper oxidases, oxygen reduction reaction, inhibition, biofuel cells, voltammetry

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SOLAR-TO-X TECHNOLOGIES AND THEIR ESSENTIAL ROLE IN A RESILIENT AND LOW-CARBON FUTURE

Gabriele Centi^{a*}, Siglinda Perathoner^a

^aUniversity of Messina (Italy) and ERIC aisbl (European Research Institute of Catalysis, Belgium), Dept. ChiBioFarAm, V.le F. Stagno D'Alcontres 31, 98166 Messina (Italy)

Abstract

Solar energy is the most abundant renewable energy source on Earth, and solar energy technologies are essential in achieving worldwide commitments towards a carbon-neutral society (1-3). However, for solar energy to be usable, it should be transformed into heat, electricity or incorporated into chemicals. The latter allows renewable energy to be stored in chemical bonds, thus enabling long-term renewable energy storage and long-distance energy transport. Developing those chemical energy vectors is crucial to replacing fossil fuels and establishing a renewable-based economy and carbon circularity (4). Chemical conversion technologies directly using solar energy, so-called Solar-to-X technologies, are central to implementing chemical energy conversion solutions.

This keynote lecture will first introduce the background aspects, the vision of the future and evolving scenario, and why solar-to-X technologies are essential in a resilient and low-carbon future. It analyses the changing energy-chemistry nexus, the drivers for a new sustainable energy scenario, a new vision for refineries, the enabling aspects towards fossil-free chemical production, approaches in defossilization and electrification of the production, and low-carbon H₂ briefly. It is highlighted, in particular, the need to turn the perspective to address these aspects (5-7).

The second part of the lecture will be focused on the features and role of artificial leaf/tree-like devices as an example of solar-to-X technologies (3, 8-13). Their feature and design, state of development and advances under development (such as artificial trees for continuous H₂ production or for making chemicals and food components from the air) will be discussed, showing how these artificial leaf/tree technologies are not a long-term dream, but a real possibility in a medium term, if enough research effort will be dedicated. This lecture is part of the activities related to EU CSA SUNER-C project 101058481 and ERC SCOPE Synergy project 810182.

Keynote: Solar-to-X; Low-carbon chemicals; Artificial leaf; Solar H₂; Air to chemicals

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ENVIRONMENT-FRIENDLY NANOCELLULOSE: CATALYSIS, SURFACE ENGINEERING, AND SUSTAINABLE EMULSIFIER APPLICATIONS

Lee Hwei Voona,*

^aNanotechnology & Catalysis Research Centre, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.

**Corresponding author: leehweivoon@um.edu.my*

Abstract

The high demand for fossil-based polymers and non-biological inorganic nanoparticles, which pose risks to human health, environment and lack sustainability, has prompted a shift towards developing materials derived from biological sources. This research focuses on creating eco-friendly nanocellulose (nanocrystalline cellulose, NCC) from natural lignocellulosic biomass, which is plentiful in Malaysia due to its active agro-forestry economy. The nanocrystalline celluloses obtained from wood and agricultural residues are low in toxicity, versatile, and biocompatible, making them suitable for various green applications, such as in food and beverages, cosmetics, personal care, hygiene, pharmaceuticals, and biomedical products.

While NCC holds significant promise as a substitute for petroleum-based resources, it faces challenges due to the intricate production process and the natural hydrophilicity of nanocellulose, which diminishes the oil-water interface interaction necessary for the development of a wide range of products. Thus, an innovative process to isolate NCC from agricultural residues through a sustainable one-pot system, followed by surface modification of NCC was developed for amphiphilic characteristics. The structural, self-assembly, and physio-chemical properties of modified NCC towards the stabilization between liquid-oil interfaces was investigated. In addition, interfacial rheology, microstructure of the emulsions, as well as particles' location (NCC & oil droplets) were conducted to explore the formulation of liquid-, gel-, and cream-based products.

The group has successfully developed several modified nanocrystalline celluloses with multiple functions, serving as natural nano-additives for a wide range of colloid stabilization or liquid/liquid dispersion formulations. This invention presents opportunities for collaboration with various industries in the production of emulsifiers, rheology modifiers, dietary fibers, lipophilic drug carriers, nutrient carriers, dietary lipid-absorbing agents, food conditioners, and more.

Keywords: Agriculture residues & wastes, catalytic process, sustainable product, bio-based nanoparticles, green application

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TOWARDS PRECISION CONTROL OF CHEMICAL REACTIONS ON METAL SURFACES FOR GREEN CHEMISTRY

Nanfeng Zheng^{a,b,*}

^aCollege of Chemistry and Chemical Engineering, State Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen, 361005, China

^bInnovation Laboratory for Sciences and Technologies of Energy Materials of Fujian Province (IKKEM), Xiamen 361102, China

*Corresponding author: nfzheng@xmu.edu.cn

Abstract

The surface and interface of solids is the place where many chemical reactions take place. How to achieve precise control of chemical reactions at solid surfaces and interfaces is a long-term challenge in heterogeneous catalysis. Although surface modification has been well documented as an important means to optimize heterogeneous catalysts, the mechanistic understanding of how surface modification manipulates heterogeneous catalysis is still severely lacking. In this presentation, we will discuss our ongoing research efforts to understand how the organic/inorganic coordinative species on metal surfaces manipulate their catalytic properties. Based on the development of new methods to construct model metal materials to resolve the molecular level structures of typical metal-organic and metal-support interfaces, we elucidate the molecular mechanisms of related interfaces in catalysis from the perspective of coordination chemistry. The understanding has been successfully applied to optimize the chemical properties of metal nanomaterials for green chemistry. The coupling of the developed techniques with renewable electricity will be discussed too.

Keywords: surface and interface coordination chemistry, Selective hydrogenation, hydrogen economy,

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CARBON NANOMATERIALS DOPED CARBON NITRIDE FOR EFFICIENT PHOTOCATALYTIC DEGRADATION OF ENVIRONMENTAL POLLUTANTS

Season S. Chen^{1,*}, Lingfeng Ouyang¹

¹*Institute of Environment and Ecology, Tsinghua Shenzhen International Graduate School, Guangdong, P.R. China, 518101*

**Corresponding author: season.chen@sz.tsinghua.edu.cn*

Abstract

Graphitic carbon nitride ($g\text{-C}_3\text{N}_4$), a prominent metal-free semiconductor photocatalyst, faces limitations due to its high exciton binding energy. Herein, our density-functional theory (DFT) and time-dependent DFT calculations revealed that the introduction of carbon dots (CD) architected a donor-acceptor interface with $g\text{-C}_3\text{N}_4$, perturbing the excited state from localized to charge transfer excited state. Synthesized via a facile thermal polymerization, CD-doped $g\text{-C}_3\text{N}_4$ ($g\text{-C}_3\text{N}_4/\text{CD}$) exhibits reduced exciton binding energy (from 41.0 to 24.6 meV). Notably, $g\text{-C}_3\text{N}_4/\text{CD-10}$ (10 wt% CD doped $g\text{-C}_3\text{N}_4$) demonstrates a 3-fold increase in the photodegradation rate ($k = 0.020 \text{ min}^{-1}$) of an emerging environmental pollutant, levofloxacin (LEV), under 10 W LED light. Enhanced photocatalytic behavior is attributed to optimized band structure and efficient charge transport, as confirmed by photophysical and photoelectrochemical analyses. This work signified the importance to manoeuvre charge transfer excited state character for efficient photocatalysis in environmental applications, offering insights to $g\text{-C}_3\text{N}_4$ -based photocatalysis via manipulating the excited state charge dynamics.

Keywords: Excited states; Carbon dots; Photodegradation; Charge transfer; Emerging contaminants

MICROPLASTICS AT THE INTERFACE: ESTUARINE CONVERGENCE, BENTHIC BIOFILMS, AND CO-POLLUTANTS-DRIVEN IMPACT

Mui-Choo Jong^{a,*}, Mengli Chen^b, Rui Yang^a

^a *Institute of Environment and Ecology, Tsinghua Shenzhen International Graduate School, Tsinghua University, Shenzhen 518055, China.*

^b *Tropical Marine Science Institute, National University of Singapore, 18 Kent Ridge Road, 119227, Singapore.*

**Corresponding author: florence.jong@sz.tsinghua.edu.cn*

Abstract

Microplastics have emerged as pervasive pollutants in aquatic ecosystems, with complex transport pathways and ecological consequences. This presentation synthesizes findings from interrelated studies to provide a comprehensive understanding of microplastic dynamics across coastal, estuarine, and freshwater environments. First, the convergence of floating microplastics at estuarine fronts, regulated by salinity gradients, highlights the role of estuarine circulation in accumulating microplastics at the land-sea interface. **The interactions between riverine inputs and tidal currents are key drivers influencing the spatial distribution of microplastics associated with the surface frontal system, suggesting an overlooked pathway** when considering the dispersal and distribution of marine plastic debris in marginal sea hotspots.¹ Second, the interactions of microplastics with resident microbiota and ambient co-pollutants at the benthic interface, including plastisphere dynamics and synergistic impact on polluted sediments underscores the importance of particle interactions in modulating microplastic fate and transport. In benthic river environments, biofilm formation selectively enriches microorganisms based on plastic type, with varying degradation outcomes, influencing long-term retention and ecological impacts. Recent work demonstrates the strong adsorption of liquid crystal monomers (LCMs) onto microplastics (1.27-1.51 mg/g), which alters their environmental behavior and impacts sediment microbial communities. **Microbial diversity and metabolic functions in sediments are significantly influenced by the presence of microplastics-LCM complexes, with potential implications for niche health and biogeochemical cycles.** Together, these studies demonstrate the interconnectedness of physical, chemical, and biological processes in shaping microplastics environmental behavior. Coastal systems act as conduits for microplastic transport, while estuarine fronts serve as temporary yet recurring hotspot, concentrating particles before potential offshore export.² This integrated perspective underscores the need for multidisciplinary approaches to tackle microplastic pollution, including advanced monitoring, predictive modeling, and targeted mitigation strategies. Crucially, sustainable plastic resource management is essential to minimize microplastic leakage into the environment.

Keywords: Microplastics, estuarine, plastisphere, liquid crystal monomers, microbial changes

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PHOTOTHERMAL CATALYTIC TECHNOLOGY FOR SOLAR FUELS PRODUCTION

Jinqiang Zhang^{a,b,*}, Hongqi Sun^a, Shaobin Wang^b

^a School of Molecular Sciences, The University of Western Australia, Perth, WA 6009, Australia

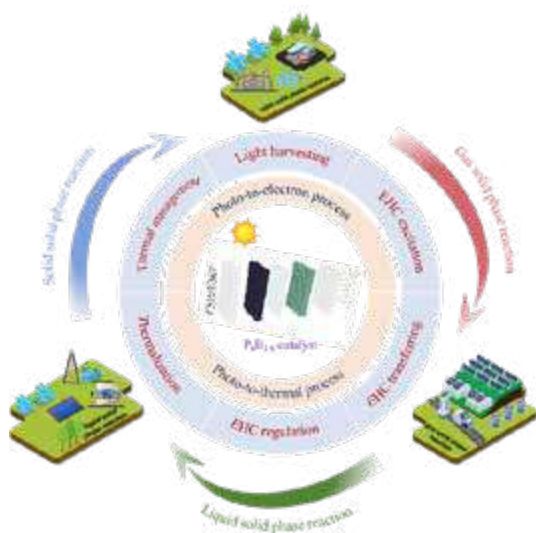
^b School of Chemical Engineering, The University of Adelaide, Adelaide, SA 5005, Australia

*Corresponding author: jinqiang.zhang@adelaide.edu.au

Abstract

Photothermal catalysis has been proposed as a promising alternative to conventional photocatalysis and thermocatalysis in the fields of energy preparation and environmental remediation, attributing to the unprecedented light harvesting efficiency and superior throughputs under moderate reaction conditions [1]. It is basically a multiple energy complementary technology integrating solar energy mediated photochemical process and solar light induced thermocatalysis. Specifically, the photo-excited energetic hot carriers via intraband or interband extinction (also called Landau damping) can directly initiate chemical reactions at much milder conditions. And the hot carriers failing to participate the redox reactions will be cooled into heat by thermalization (also named Ohmic damping) [2]. The photo-excited hot carriers can reduce the reaction barrier and improve the reaction selectivity, while the photo-generated internal heat can thermodynamically accelerate reaction rates and ginger up the sluggish hot carriers. Therefore, photothermal catalysis has compensated the disadvantages of photocatalysis and thermocatalysis, and significantly boosted the reaction rates to a level of industrialization by taking advantage of full-spectrum solar light, showing significant potentials on large-scale production of solar fuels [3]. Here, we present our ongoing researches in harnessing the full spectrum solar energy using the photothermal catalytic strategy to drive CO₂ reduction with alkane or hydrogen. Using solar energy to catalytically reduce CO₂ and upgrade conventional fossil fuels has the potential to convert the waste of CO₂ into high value-added chemical fuels and feedstocks in a clean and sustainable manner, allowing the dual opportunity to store the intermittent renewable energy as well as closing the anthropogenic carbon cycle.

Keywords: photothermal catalysis, solar fuels, hot carriers, localized thermal, active sites



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SYNTHESIS, CHARACTERIZATION, AND APPLICATIONS OF MOLECULARLY IMPRINTED POLYMERS FOR SELECTIVE EXTRACTION OF ANTIRETROVIRAL DRUGS IN WATER: STEPS TOWARDS ATTAINING GREEN SYNTHETIC ROUTES

Lawrence M. Madikizela

University of South Africa, Johannesburg, South Africa

madiklm@unisa.ac.za

Abstract

Recently, the occurrence of antiretroviral drugs in South African waters has been reported ¹. In recent years, through the non-target analytical approach using solid-phase extraction and ultra-high-performance liquid chromatography-quadrupole time-of-flight-mass spectrometry analysis, 47 pharmaceuticals were detected in a South African river with 31 drugs being found present for the first time, while 7 were not recognized as South African medications ². An antiretroviral drug, efavirenz was among the detected pharmaceuticals ². To gain more insights into the presence of antiretroviral drugs in water, the synthesis and characterization of molecularly imprinted polymers (MIPs) for their selective extraction in water was investigated. Green monomers such as ionic liquids and deep eutectic solvents for molecular imprinting were explored in this case. Notably, aliquat 336 was used as the functional monomer to produce a MIP that selectively recognized abacavir in aqueous samples (maximum adsorption capacity of 5.98 mg/g). Upon application in environmental monitoring, the detected concentrations of abacavir in wastewater influent, effluent, and estuarine water were 41, 24 and 22 µg/L, respectively. Furthermore, deep eutectic solvents were used as functional monomers to synthesize MIPs for emtricitabine. The fate of pharmaceuticals in the South African environment is not yet well-understood with recent work showing the occurrence of these drugs in seawater.

Keywords: Green analytical chemistry; Molecular imprinting; Selective extraction; Adsorption

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DETERMINATION OF PESTICIDE RESIDUES IN BEANS USING QUECHERS TECHNIQUE COUPLED TO GAS CHROMATOGRAPHY-MASS SPECTROMETRY: MULTIVARIATE OPTIMIZATION OF CEN AND AOAC METHODS

Abdulra'uf, L. B.^{a,b*}, Junaid, A. M.^{a,c}, Lawal, A. R.^d, Ibrahim, H. B.^e, Tan, G. H.^b,

^aDepartment of Chemistry and Industrial Chemistry, Faculty of Pure and Applied Sciences, Kwara State University
Malete, P. M. B. 1530, Ilorin, Nigeria

^bDepartment of Chemistry, Faculty of Science, University of Malaya, Kuala Lumpur, Malaysia

^cDepartment of Chemistry, School of Science, Kwara State College of Education, P. M. B. 1525, Ilorin, Nigeria

^dDepartment of Plant and Environmental Biology, Faculty of Pure and Applied Sciences, Kwara State University
Malete, P. M. B. 1530, Ilorin, Nigeria

^eDepartment of Integrated Science, School of Sciences, Kwara State College of Education, P. M. B. 1525, Ilorin,
Nigeria.

*Corresponding author: abdulrauf.bola@kwasu.edu.ng

Abstract

The use of pesticides has led to environmental pollution and posed a global health risk, since they remain as residues on foods. Beans one of the most widely cultivated crop in Africa, and susceptible to attack by insects both on field and during storage, leading to the application of pesticides to control pests' infestation. However, misuse of these chemicals by farmers on beans has resulted in the rejection of beans exported to European countries, due to the presence of pesticide residues at concentrations higher than the maximum residues levels (MRLs). In this study, the effectiveness of the Association Official Analytical Chemists (AOAC) Official Method and the European Committee of Standardization (CEN) Standard Method, were determined using multivariate approach for the analysis of organochlorine pesticide residues in 6 varieties of beans samples. The significance of factors (mass of sample, volume of acetonitrile, mass of magnesium sulphate, sample pH, centrifugation time and speed) affecting the efficiency of extraction was estimated using Plackett-Burman design, while central composite design was used to optimize the significant factors. The following optimum factors were subsequently used for method validation, recovery tests, and real sample analysis: 4 g of sample sludge (1:1 v/v), 10 mL of acetonitrile, 4.45 g of MgSO₄, and 5 min of centrifugation at 5000 rpm. The figure of merit of analytical methodology estimated using matrix-matched internal standard calibration method gave linearity ranging from 0.25 to 500 µg/kg, with correlation coefficient (R²) greater than 0.99, the recovery ranged from 75.55 to 110.41 (RSD = 0.70–16.65), with LOD and LOQ of 0.23–1.77 µg/kg and 0.76–5.88 µg/kg, respectively.

Keywords: GC/MS, Multivariate, Pesticide residues, QuEChERS technique, Sample preparation

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GROUP II PROMOTERS FOR SULFUR CONTAMINATED Ni/ γ -Al₂O₃ CATALYSTS IN CO₂ HYDROGENATION

Hasliza Bahruji^{a,*}, Amira Afra Adam^a

^a*Centre of Advanced Material and Energy Sciences, Universiti Brunei Darussalam, Jalan Tungku Link, Gadong, Brunei Darussalam*

**Corresponding author: hasliza.bahruji@ubd.edu.bn*

Abstract

Catalyst with a high tolerance to sulfur is important when using CO₂ feedstock contaminated with H₂S impurities. Sulfur has high affinity towards transition metal, strongly chemisorbed on the active metal sites. Sulfur impurities deactivates Ni on alumina when presence in the reaction gases [1]. This study elucidates the susceptibility of sulfur contaminated γ -Al₂O₃ to form NiAl₂O₄ species under hydrogenation. The presence of residual sulfur in the form of Al₂(SO₄)₃ was hypothesised to have caused Ni to change into NiAl₂O₄, in which it decreased the Ni⁰ sites for hydrogen dissociation. During the reduction of the catalysts, -SO₄ reduction generates oxygen vacancy on Al₂O₃. The proximity with Ni²⁺ allowed the formation of NiAl₂O₄ species. The inhibit formation of Ni⁰ is detrimental for the formation of formate intermediates during CO₂ hydrogenation. *In-situ* DRIFTS analysis revealed that sulfur impurities caused CO₂ hydrogenation via CO₂ dissociation into CO, followed by the subsequent hydrogenation to CH₄. A facile route to improve catalytic activity of sulfur contaminated catalysts stability was investigated using metal oxides promoters. The formation of the BaAl₂O₄ phase seems to take place by the dissolution of Ba²⁺ ions into the γ -Al₂O₃ lattice. The doping of alumina with Ba leads to a decrease of NiAl₂O₄ content in the corresponding catalyst, further improving the efficiency of Ni⁰ as hydrogen dissociation sites during the methanation reaction.

Keywords: : γ -Al₂O₃, methanation, promoter, sulfur, nickel

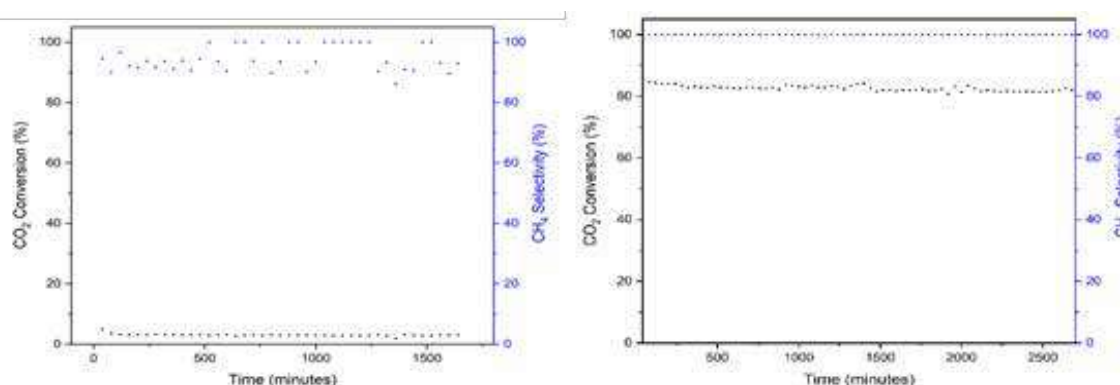


Fig 1. CO₂ conversion and CH₄ selectivity on Left: sulfur contaminated Ni/Al₂O₃; Right: Barium promoted Ni/Al₂O₃

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DEVELOPMENT OF HYPER-CROSS-LINKED RESIN FOR WATER REMEDIATION EFFORT FROM A VARIETY OF POLLUTANTS

Mochamad Lutfi Firmansyah^{a,*}, Nisar Ullah^{a,b}

^a Interdisciplinary Research Center for Refining & Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

^b Chemistry Department, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia

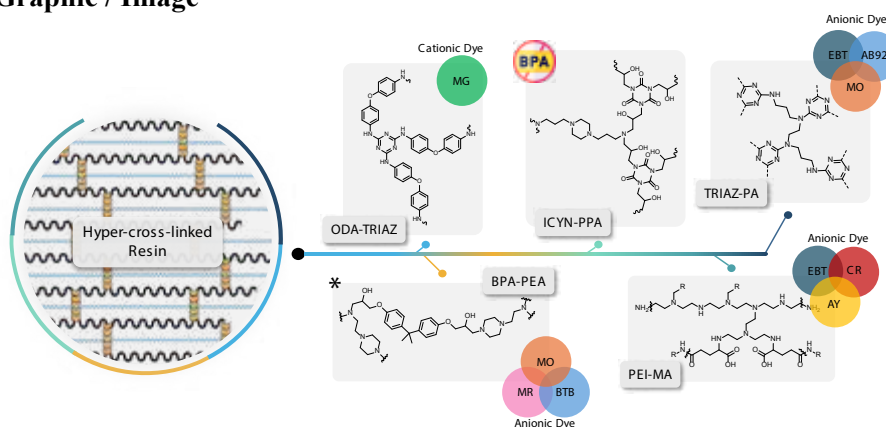
*Corresponding author: mochamad.firmansyah@kfupm.edu.sa

Abstract

Over the last few decades, global water consumption has doubled due to intensive agriculture, industry, and domestic use¹. Thus, access to clean drinking water becomes one of the focuses of the United Nation's SDGs². Thus, the remediation of water bodies is of paramount importance. Herein, we disclose the synthesis of a novel hyper-cross-linked resin, dubbed BPA-PEA, for the adsorptive removal of colorant from an aqueous solution³. Moreover, various cross-linked resins that have been synthesized and utilized in water remediation efforts by our group will be discussed as well⁴. Hyper-cross-linked resins are pivotal due to the advantages of fine-tuning their porosity, surface functionalities, and ease of regeneration under milder conditions. BPA-PEA was achieved from the condensation of bisphenol A diglycidyl ether and 2-piperazinoethylamine. The hyper-cross-linked resin showed a remarkable adsorption capacity at over 200 mg/g for three types of anionic dyes. Density Functional Theory (DFT) simulations indicate a spontaneous binding process, with binding order closely aligned with the experimentally observed order. The linearity and smaller size of the carboxylate group facilitate its encapsulation in the resin-dye complex, enhancing molecular matching and interactions with the resin. The adsorption mechanism is mainly governed by electrostatic interaction between the dyes and adsorbent. However, other adsorptive mechanisms, such as H-bonding interactions, hydrophobic interactions, or π - π interactions, were also involved. Furthermore, a comprehensive analysis of hyper-cross-linked resin performance dealing with other types of pollutants showcased the capability of the adsorbent in the field of water remediation.

Keywords: hyper-cross-linked resin, adsorption, organic pollutant, water remediation

Graphic / Image



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MICROPLASTICS AS AN EMERGING ENVIRONMENTAL POLLUTANT IN AGRICULTURAL SOILS: CURRENT UNDERSTANDING FROM MALAYSIA

Sarva Mangala Praveena^{a,*}, Shyamala Devi Shanmugam^a, Muhammad Aiman Fahim Ishak Hisham^a, Ayu Lana Nafisyah^b,

^aUniversiti Putra Malaysia

^b Universitas Airlangga

*Corresponding author: smpraveena@upm.edu.my

Abstract

Microplastics (plastic particles <5 mm) is of particular concern due to its small size and deleterious impacts on both marine and terrestrial systems. However, microplastics accumulation in soil was found 4 to 23 times greater by mass relative to marine systems. Moreover, microplastics that enter the soil environment may persist long-term due degradation difficulty¹. Similar to the global trend, the majority of microplastics studies in Malaysia have concentrated on the marine environment, while understanding of this pollution in terrestrial environments, particularly in soil, is rather limited². Thus, this study aims to explore microplastics pollution sources in terrestrial environment particularly from agricultural soil from Malaysia. So far, the mean number of microplastics particles found in the agricultural soils were 2.1 to 5.3 particles/kg, which corresponds with the plastic usage intensity at these farms. Microplastics particle sizes ranged from 16.7 to 3261 μm , attributing to their extensive breakdown processes. The microplastics particle shapes (film, fibre, and fragment) and colours (black, white, red and blue) from the soil samples reflected the type of plastics products used and unmanaged plastics waste at these farms. Plastic nets, mulching films, and unmanaged plastics waste constitute the microplastics sources at these farms^{3,4}. Thus, extensive studies are needed to further understand the effects of these microplastic particles in soil environment. Further initiatives from scientific communities and actions from regulatory bodies are also needed to minimize this pollution in soil environment.

Keywords: Microplastics; Pollution; Agricultural Soil; Malaysia



Microplastics particles found in agricultural soil samples

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PHOTOREFORMING OF LIGNOCELLULOSE OVER SINGLE-ATOM FE DISPERSED POLYMERIC CARBON NITRIDE HOMOJUNCTIONS

Can Xue^{a*}

^a*School of Materials Science and Engineering, Nanyang Technological University, Singapore.*

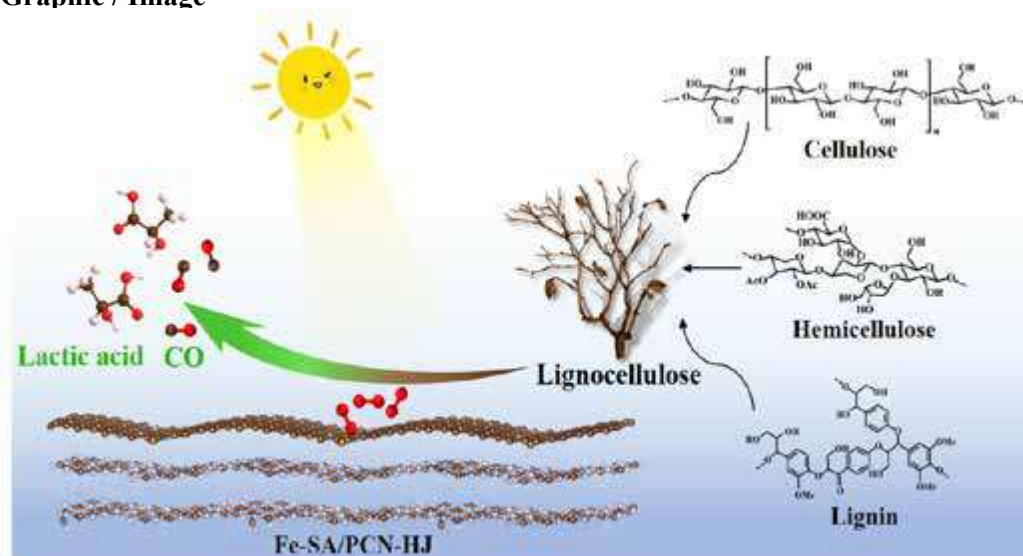
^{*}*Corresponding author: cxue@ntu.edu.sg*

Abstract

Photoreforming of lignocellulose into valuable fuels and chemicals represents an environmentally friendly and energy-saving technology. We present the construction of Fe-doped polymeric carbon nitride homojunction (PCN-HJ), in which Fe single atoms are confined to PCN-HJ surface, for highly efficient photocatalytic reforming of lignocellulose into CO and lactic acid. Experimental investigations and theoretical calculations reveal that the homojunctions and dispersed Fe atoms on the surface greatly improve the separation efficiency and transport of photogenerated charge carries. Driven by the internal electric field across the entire junction, the photogenerated electrons can rapidly migrate from the bulk to the surface, leading to enrichment of surface electrons at the dispersed Fe-N₄ sites. In addition, the Fe-N₄ sites optimize the adsorption and activation of molecular oxygen and facilitate electron transfer to the adsorbed molecular oxygen, thereby promoting the formation of reactive oxygen species for lignocellulose photoreforming. As such, the Fe-dispersed PCN-HJ exhibits ultrafast CO generation with high yield of lactic acid via photoreforming of fructose. Further, we demonstrate that this Fe-dispersed PCN-HJ shows universal applicability for photoreforming of various types of lignocellulosic biomass.¹

Keywords: Photocatalysis; lignocellulose biomass; solar fuels; carbon nitride; single-atom catalyst

Graphic / Image



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EXPLORING THE POTENTIAL OF FRESHWATER ALGAE FOR ACTIVE COMPOUND EXTRACTION AND ENVIRONMENTAL MONITORING

Zuzanna Piotrowicz^{a,*}, Łukasz Tabisz^a, Bogusława Łęska^a, Radosław Pankiewicz^a

^aAdam Mickiewicz University, Poznan, Poland

*Corresponding author: zuzanna.piotrowicz@amu.edu.pl

Abstract

Algae have long been recognized as a valuable source of active compounds, nutrients, and biofuels, with marine species typically being the primary focus of research. However, freshwater algae, which dominate inland reservoirs in many European countries, also present a significant biomass that could be equally promising as a source of bioactive ingredients.

A stepwise extraction process was applied to isolate distinct fractions of active compounds for further analysis. Using solvents of varying polarity (hexane, ethanol, and water), we separated lipids, carotenoids, polyphenols, polar dyes, and sulphated polysaccharides. Lipids, for example, can be used in biodiesel production. Special attention was given to phenolic compounds, which possess antioxidant properties and can provide valuable information about environmental conditions. Algae secrete polyphenols in response to stress, and their concentration in both the thallus and surrounding water can serve as an ecological monitoring tool.

Complementary semi-quantitative colorimetric methods were used to create simplified profiles of antioxidant compounds, including phenolic compounds. Additionally, the lipid fraction was analyzed to enrich the profile with carotenoids and fat-soluble vitamins. Furthermore, sulphated polysaccharides, isolated for the first time from freshwater algae by our team, have potential applications in the pharmaceutical, food, and cosmetic industries.

Keywords: Freshwater algae, Polyphenols, Sulphated polysaccharides, Bioactive compounds from algae, Colorimetric assays

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WHAT'S LURKING IN TYRES? CHEMICAL INSIGHTS INTO RECYCLED RUBBER

Divina Navarro^a, Anna Heitz^b, Cynthia Joll^b, Prashant Srivastava^a, Mike Williams^a, Greg Davis^c,
Naomi J Boxall^c

^a*CSIRO Environment, Private Bag 2, Glen Osmond SA 5064, Australia*

^b*Curtin Water Quality Research Group, School of Molecular and Life Sciences, Curtin University, Bentley
WA 6102, Australia*

^c*CSIRO Environment, Private Bag No. 5, Wembley WA 6913, Australia*

^{*}*Corresponding author: divina.navarro@csiro.au*

Abstract

Australia's ban on tyre exports has created both challenges and opportunities for circular economy applications of recovered rubber materials. However, emerging chemicals of concern, such as 6PPD-quinone (6PPD-Q) and hexamethoxymethyl-melamine (HMMM), may impact reuse potential due to ecotoxicological risks. Limited data exist on the chemical composition and potential hazards of end-of-life (EOL) tyres in Australia's unique environment. This study aimed to build quantitative datasets on the chemical composition of Australian EOL tyres and e-waste streams. Targeted analyses were conducted on recycled rubber products, using accredited laboratories to screen for known contaminants. While total chemical content aligned with literature values (e.g., 79.6% carbon, 1.2% sulfur), specific compounds of interest—including 6PPD-Q and HMMM—were detected at mg/kg levels. Leaching tests using the Australian Standard Leaching Procedure (ASLP) identified HMMM as the most readily leachable compound, consistent with its frequent detection in urban runoff. Despite samples being classified as homogenous, metal concentrations varied, suggesting a need for increased sample frequency to account for intrinsic variability. The study also indicated that many organic compounds remained unidentified, highlighting the need for non-targeted screening methods. While findings were generally consistent with known data, the small sample size (n=3) limits broader conclusions. Expanding chemical characterisation efforts and developing comprehensive screening approaches will be critical to supporting safe resource recovery and circular economy strategies for rubber materials in Australia.

Keywords: tyres, 6PPD-Q, contaminants, chemicals of concern, end of life

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OXIDATIVE DEGRADATION OF VENLAFAXINE IN A 3D-PRINTED LAB-SCALE ELECTROCHEMICAL CELL

Martin Šefčík^{a,*}, Simona Baluchová^a, Anna Kubíčková^a, Jan Fischer^a

^aCharles University, Faculty of Science, Department of Analytical Chemistry, Albertov 6, 128 00, Prague 2, Czech Republic

*Corresponding author: martin.sefcik@natur.cuni.cz

Abstract

Water pollution by pharmaceuticals is a growing concern, as these bioactive compounds persist in the environment despite conventional wastewater treatment process¹. Even at trace concentrations, they pose potential health risks². Electrochemical advanced oxidation processes (EAOPs), which generate reactive species such as hydroxyl radicals, present a promising eco-friendly solution for the complete degradation of these contaminants. Among electrode materials, boron-doped diamond (BDD) anodes stand out due to their exceptional stability, corrosion resistance, and high radical generation efficiency³. This study investigates the oxidative degradation of venlafaxine, a frequently detected pharmaceutical and emerging environmental pollutant, using a newly designed lab-scale electrochemical cell and a free-standing BDD electrode⁴. Venlafaxine was selected due to its widespread use as an antidepressant, its ranking as the 21st most frequently detected pharmaceutical in the world's rivers⁵, and its resistance to conventional treatment processes⁶. To optimize degradation efficiency, a novel 3D-printed electrochemical cell was designed and fabricated via stereolithography, allowing for customizable and precise configurations tailored to specific experimental needs⁷. Lab-scale electrochemical cells play a crucial role in evaluating the feasibility and efficiency of EAOPs before scaling up to high-volume water treatment applications. In this study, the dual-function cell was specifically developed to facilitate both the detection and degradation of venlafaxine. The degradation process was monitored using a fast voltammetric technique, as well as Ultra-High Performance Liquid Chromatography-Mass Spectrometry (UHPLC-MS), which provided both quantification of venlafaxine and identification of its degradation products.

Keywords: 3D-printed lab-scale electrochemical cell, boron-doped diamond (BDD) anode, oxidative degradation, venlafaxine, water treatment process

Acknowledgements

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AMINE-FUNCTIONALIZED HIERARCHICALLY POROUS PORPHYRIN-BASED METAL –ORGANIC FRAMEWORKS FOR HIGHLY ENHANCED DIRECT AIR CAPTURE OF CO₂

Shanshan Shang^{a*}, Xinyu Chen^a, Jinhai Leng^a, Fengying Ma^a

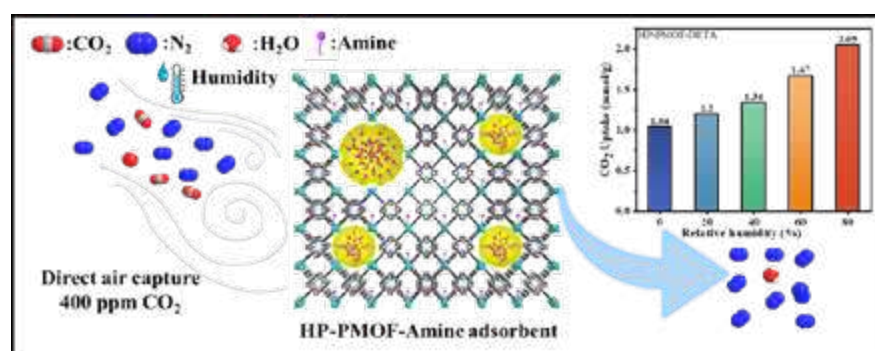
^a*School of Environment and Energy, South China University of Technology, Guangzhou, China.*

^{*}*Corresponding author: ssshang@scut.edu.cn (S. Shang)*

Abstract

Direct air capture (DAC) of carbon dioxide (CO₂) has gained prominence as a vital “negative carbon emission technology” for achieving carbon neutrality, particularly following the “1.5 Degree Scenario” presented at COP21.¹ To enable large-scale DAC, developing solid porous adsorbents that efficiently capture CO₂ from the atmosphere (approximately 400 ppm concentration) is essential. Among various adsorbents, amine-functionalized metal-organic frameworks (MOFs) have shown exciting potential as adsorbents for atmospheric CO₂ capture.² However, the intrinsic microporosity of many MOFs restricts amine loading and uniform dispersion, diminishing CO₂ adsorption efficiency. In this study, we synthesized a series of hierarchically porous porphyrin-based MOF (HP-PMOF) featuring high-density defects and a combination of micro- and meso- and macropores. The HP-PMOF was subsequently functionalized with short-chain alkyl amines (diethylenetriamine (DETA) and tetraethylenepentamine (TEPA)) and polyamines (polyethyleneimine (PEI)) to form HP-PMOF-Amine composites. Evaluations of these adsorbents demonstrated significantly enhanced CO₂ capture performance in DAC applications. Static CO₂ adsorption isotherms revealed that HP-PMOF-DETA achieved the highest CO₂ uptake of 1.40 mmol g⁻¹, representing increases of 140 and 20 times over unmodified PMOF and HP-PMOF, respectively. Dynamic DAC performance measurements showed that HP-PMOF-DETA maintained 84% regeneration efficiency after ten cycles under 400 ppm CO₂. Breakthrough tests demonstrated enhanced CO₂ adsorption capacity across varying relative humidity (0-80%) compared to dry conditions. Mechanistic insights from *in-situ* infrared Fourier transform spectroscopy (DRIFTS) studies indicated that, under dry conditions, physisorption and chemisorption synergistically occur between CO₂ and amine groups of DETA, forming carbamate or carbamic acid species. Under humid conditions, water facilitated CO₂ adsorption by promoting the conversion of ammonium carbamate to bicarbonate. This work underscores the significant potential of amine-functionalized hierarchically porous MOFs for advancing the efficacy of DAC technologies.

Keywords: Hierarchical pore, Metal–organic frameworks, Direct Air Capture, Amine functionalization



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MNO NANOPARTICLES FOR CO₂ CAPTURE: INFLUENCE OF NANOPARTICLE SIZE ON ADSORPTION PERFORMANCE

Syawal Mohd Yusof ^{a,b}, Azizul Hakim Lahuri^{a,*}, Nurul Asikin Mijan^{2b}, Siti Sarahah Sulhadi^{1a},

^a*Department of Science and Technology, Universiti Putra Malaysia Bintulu Campus, Nyabau road, P.O. Box 396, 97008 Bintulu, Sarawak, Malaysia.*

^b*Department of Chemical Science, Faculty of Science and Technologi, Universiti Kebangsaan Malaysia, 43600, Bangi, Selangor, Malaysia.*

**Corresponding author: azizulhakim@upm.edu.my*

Abstract

The increasing concentration of carbon dioxide (CO₂) in the atmosphere has necessitated the development of effective carbon capture technologies. Manganese oxide (MnO) nanoparticles have emerged as promising materials due to their high surface area, tunable porosity, and excellent redox properties. This study investigates the effect of MnO nanoparticle size on CO₂ capture efficiency. MnO nanoparticles were synthesized using a controlled precipitation method by varying the concentration of potassium permanganate (KMnO₄), leading to different particle sizes labeled as MnO-1, MnO-3, MnO-5, and MnO-7. The synthesized nanoparticles were characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), Brunauer-Emmett-Teller (BET) analysis, and temperature-programmed desorption (TPD-CO₂) to evaluate their structural, morphological, and adsorption properties. The results revealed that smaller MnO nanoparticles exhibited enhanced CO₂ capture capacity due to their higher surface area and microporosity. MnO-1, which had the smallest crystallite size and highest surface area (120.4 m²/g), demonstrated the highest CO₂ adsorption capacity of 465.14 cm³/g. Conversely, larger MnO particles (MnO-7) had lower surface areas, reduced oxygen vacancies, and fewer active adsorption sites, resulting in diminished CO₂ capture performance. The CO₂ chemisorption capacity followed the trend: MnO-1 > MnO-3 > MnO-5 > MnO-7. The enhanced performance of MnO-1 was attributed to its well-developed microporous structure and abundant oxygen vacancies, which facilitated strong CO₂ binding. This study highlights the significant impact of nanoparticle size on CO₂ adsorption performance, demonstrating that optimizing MnO synthesis conditions is crucial for enhancing carbon capture efficiency. These findings provide valuable insights into the development of efficient MnO-based adsorbents for industrial CO₂ capture applications.

Keywords: MnO nanoparticles, CO₂ capture, adsorption capacity, oxygen vacancies, nanoparticle size.

PREPARATION AND TESTING METHODS OF NANO UREA FOR AGRICULTURAL APPLICATIONS

Shrikant P Aherkar^{a,*}, Surykant B. Sapkal^a

^a *University Department of Basic and Applied sciences (Chemistry), MGM University, Chatrapati Sambhaji Nagar, Maharashtra-431001, India.*

**Corresponding author: shreeaherkar@gmail.com*

Abstract

The population is increasing constantly and touched up to 7.37 billion, population in India almost equivalent to 1.3 billion and population in the world will reach around 6 to 9 billion people by 2050. In worry of supplying food to such a huge population there must be novel technology giving extra yield in short phase (1). Agricultural productivity is decreasing due to reduction of cultivable land, shortage of proper nutrient supply, decline of soil health and organic matter, disease incidence, attack of insects and pests, and more importantly ineffective fertilizer management (2). The overdosage of chemical fertilizers without taking any remedial measures of soil testing has contaminated almost every part of our ecosystem, leading to the most devastating effects of soil, water, land, and air pollution (3). Nanoparticles (NPs) fertilization is an essential approach employed to mitigate the adverse impacts of soil pollution resulting from excessive utilization of chemical fertilizers. This method facilitates the slow release of essential nutrients while simultaneously reducing both biotic and abiotic stress experienced by plants.

Multiple products are commercially available as Nano fertilizer in India and other countries. Most of the research and commercial products around nano nutrients are based on using natural or naturally derived nano carriers. In our study we used synthetic nano carriers and focused on the following aspects –

1. Formulation of nano Urea at different concentrations.
2. Testing results using Differential Light Scattering (DLS) and Zeta – potential etc. advance technology.
3. Data comparison against existing market benchmarks.

As a result, we achieved physically stable Nano Urea formulations at different concentrations and the way forward in this study is to test these formulations in the field.

Keywords: Nano nutrients, Nano fertilizer, Nano urea, Differential Light Scattering (DLS), zeta potential

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QUANTITATIVE SPECIATION OF ARSENIC, CHROMIUM AND MERCURY IN WATER AND RIVER SEDIMENTS

Abayneh Ataro Ambushe^{a*}

^aDepartment of Chemical Sciences, University of Johannesburg, P.O. Box 524, Auckland Park 2006, Johannesburg, South Africa

*Corresponding author: aambushe@uj.ac.za

Abstract

Speciation of arsenic (As), chromium (Cr) and mercury (Hg) in water and river sediments serves as a vital tool for assessing water quality since the actual toxicity, mobility, bioaccumulation, and reactivity of As, Cr and Hg depend on their chemical forms. In this study, microwave assisted extraction and ultrasonic extraction methods were used to achieve a safe, simple, and fast method for quantification of different chemical species of As, Cr and Hg in river sediments. Total concentrations of these elements in water and river sediments were determined by inductively coupled plasma-mass spectrometry (ICP-MS), whereas speciation analyses were conducted by high performance liquid chromatography (HPLC) hyphenated to ICP-MS. Herein discussion will be focused on the following points with the objective of developing efficient analytical methods for speciation analysis of As, Cr and Hg in water and river sediments.

1. Synchronous extraction and quantitative speciation of As and Cr in river sediments ¹
2. Simultaneous quantitative speciation of As and Cr in water ²
3. Speciation and bioavailability of Hg in river sediments ³

The developed analytical methods were applied for quantitative speciation of As, Cr and Hg species in water and river sediment samples. The effects of industrial pollution and mismanagement of municipal wastewater will be discussed. A thermo-desorption studies of Hg in river sediments using a Zeeman direct Hg analyser to investigate the behaviour of Hg release from sediments will also be discussed.⁴

Keywords: arsenic, chromium, mercury, HPLC hyphenated to ICP-MS, quantitative speciation, river sediments, water

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Fe-CONTAINING NATURAL BENTONITES FOR THE CATALYTIC DECONTAMINATION OF HIGHLY HAZARDOUS PHOSPHORUS AND SULFUR POLLUTANTS

Sholpan Nazarkulova^{a,b}, Stefano Econdi^a,
 Mukhambetkali Burkitbayev^b, Matteo Guidotti^{a,*}

^aCNR-SCITEC, Institute of Chemical Sciences and Technologies, Milan, Italy.

^bAl-Farabi Kazakh National University, Almaty, Kazakhstan.

*Corresponding author: matteo.guidotti@scitec.cnr.it

Abstract

This study explores the use of natural clay minerals as sustainable and cost-effective sorbents for the decontamination of environmentally hazardous materials. As decontamination catalysts, mineral bentonite clays from Kazakhstan origin were used. The total reserve of bentonite clay in Kazakhstan is more than 150 million tons, main deposits being located in South and East Kazakhstan [1]. There are several research about using bentonite (Ben) as an adsorbent for wastewater treatment. The introduction of redox-active catalytically active sites into the interlayer space have already proved to produce a sorbent with marked catalytic oxidative and hydrolytic properties for the selective conversion of hazardous organophosphorus and organosulfide compounds into harmless products [2].

By cationic exchange with Fe(II) and Fe(III) salts ($\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ and $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$), Fe(II)-Ben and Fe(III)-Ben were obtained, respectively. These solids after calcination treatment (O_2 , 200°C , 2h) gave rise to Fe(II)-Ben-C and Fe(III)-Ben-C catalysts. They were used as heterogeneous catalysts for the oxidative degradation of two model hazardous contaminants, CEES, DMMP, and an obsolete agrochemical, paraoxon (Fig. 1), in the presence of aqueous H_2O_2 .

As a result, we have achieved *ca.* 99% and 75% of degradation of CEES with Fe(III) and Fe(II) modified bentonites, respectively, under extremely mild conditions (room temperature and pressure) in 24 h.

Keywords: bentonite clays, heterogeneous catalysis, sorption, modification methods

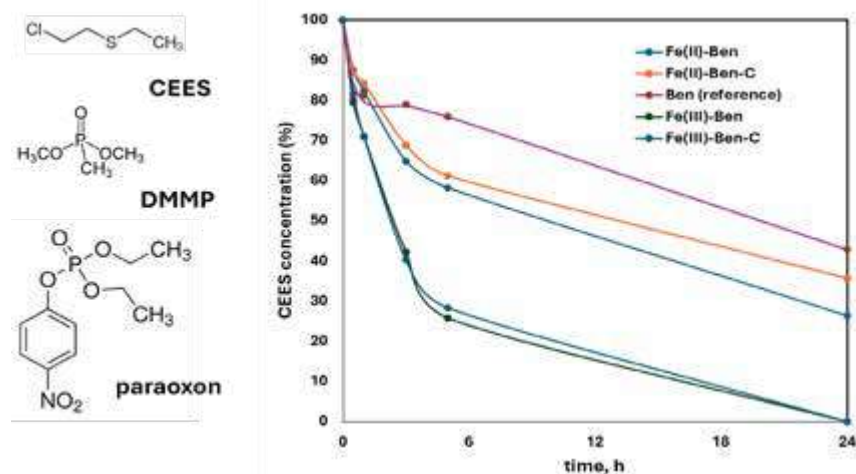


Figure 1. Schemes of CEES, DMMP and paraoxon (left). Degradation profile vs. time of CEES, in the presence of Fe-Ben catalysts; reaction conditions: batch glass reactor, 298 K, 1 bar, initial $[\text{CEES}] = 13.7 \text{ mM}$, $\text{CEES}:\text{H}_2\text{O}_2$ 1:5 ratio, AcOEt solvent.

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UNRAVELING THE ROLE OF OXYGENATED FUNCTIONAL GROUPS IN CARBON-BASED MATERIALS FOR SELECTIVE H₂O₂ ELECTROGENERATION

Taynara Oliveira Silva^{a,b,c,*}, G  ssica de Oliveira Santiago Santos^c, Marcos Roberto de Vasconcelos Lanza^c, Lu  s Augusto Martins Ruotolo^b, Frank Marken^a

^a University of Bath, Chemistry Department, United Kingdom.

^b Federal University of S  o Carlos, Chemical Engineering Department, Brazil.

^c University of S  o Paulo, Chemistry Department, Brazil

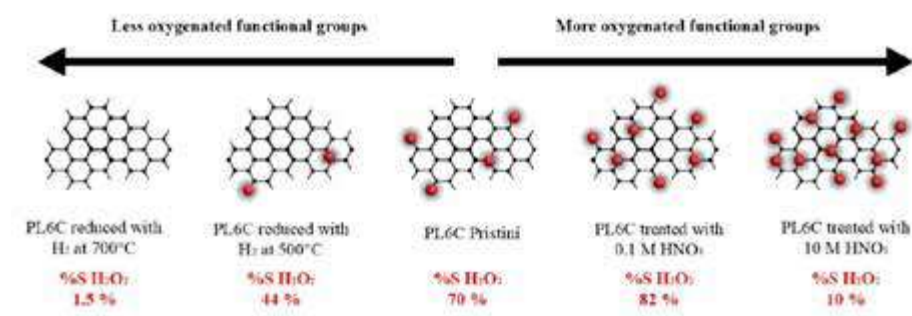
*Corresponding author: taynaraos1994@alumni.usp.br

Abstract

The selective electrogeneration of hydrogen peroxide (H₂O₂) via the two-electron oxygen reduction reaction (2e⁻ ORR) is an essential element of sustainable technologies for advanced oxidation processes^[1]. Carbon-based materials have shown great promise in this application; however, the mechanistic role of oxygenated functional groups in modulating selectivity remains poorly understood^[2]. In this frame, the present work addresses this critical knowledge gap by systematically exploring both the removal and addition of functional groups on Printex L6 carbon (PL6C), a material recognized for its intrinsic H₂O₂ selectivity^[3]. Thermal reduction treatments (500  C and 700  C) were employed to remove surface oxygenated groups, while controlled oxidative treatments using nitric acid (0.1 M and 10 M) were used to increase their density. Electrochemical analysis revealed that reducing the oxygenated groups diminished selectivity for H₂O₂, whereas moderate functionalization (0.1 M HNO₃) enhanced it. Strikingly, excessive functionalization (10 M HNO₃) led to a decline in selectivity, highlighting an optimal density of functional groups that balances active site exposure and electronic stability.

This comprehensive investigation provides unprecedented insights by correlating surface chemistry with H₂O₂ electrogeneration performance. Importantly, these modifications preserved the structural and morphological integrity of PL6C, isolating the influence of surface chemistry on the 2e⁻ ORR pathway. The findings offer a robust foundation for the rational design of next-generation electrocatalysts, capable of achieving both high efficiency and selectivity for H₂O₂ production. By elucidating the interplay between oxygenated groups and ORR selectivity, this work not only advances the fundamental understanding of carbon-based materials but also paves the way for scalable, sustainable solutions in green chemistry. Its novelty and practical relevance make it a significant contribution to the field of electrochemical technologies.

Keywords: Hydrogen Peroxide, Carbon, Selectivity, Functional Groups, Electrosynthesis.



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INFLUENCE OF DRYING AND EXTRACTION TECHNIQUES ON CARRAGEENAN PROPERTIES AND PHYTOCHEMICAL CONSTITUENTS OF *Kappaphycus striatus*

Nurwadini Fifiana Abdul Razak @ Achil^a, Nazirah Minggu^a, Sri Hilma Siregar^b, Hasmadi Mamat^c, Mohd Hafiz Abd Majid^a and Mohd Sani Sarjadi^{a*}

^aFaculty of Science and Natural Resources, Universiti Malaysia Sabah, Jalan UMS, 88400 Kota Kinabalu, Sabah, Malaysia.

^bProdi Kimia, FMIPA dan Kesehatan Universitas Muhammadiyah Riau (UMRI), Jalan Tuanku Tambusai, Pekanbaru, 28294 Riau, Indonesia

^cFaculty of Food Science and Nutrition, Universiti Malaysia Sabah, Jalan UMS, 88400 Kota Kinabalu, Sabah, Malaysia.

*Corresponding author: msani@ums.edu.my

Abstract

This research is performed to analyse the effects of different drying and extraction methods to the carrageenan and phytochemical of two varieties of *K. Striatus* which are the red and green *K. striatus*. Furthermore, the comparative study of the seaweed was also carried out based on the moisture content, functional group and the antioxidant assay (DPPH). There are two drying methods used which are oven drying and freeze drying. There are also two extraction methods used which are Hot-Water Extraction and Ultrasound-Assisted Extraction, which are used to extract carrageenan and phytochemical compounds respectively. After all sample preparation and extraction are done, the characterization of the extracts was performed. The moisture content for all dried samples is below 10%, while the oven dried red *K. Striatus* have the highest carrageenan yield which is 41.6%. The Hot-Water Extraction is able to extract kappa-carrageenan which can be seen based on the Fourier transform infrared spectroscopy (FTIR) spectra and there are band around 850 cm⁻¹ value. The green *K.Striatus* has the highest total phenolic content (TPC) (8.210 ± 1.916 mg GAE/g DS) and Radical Scavenging Activity (45.39 ± 4.411 %) while the red *K. Striatus* has the highest total flavonoid content (0.444 ± 0.008 mg QUE/g DS). Thus, different drying and extraction methods do effect the carrageenan yield and phytochemical content in the red and green *K.Striatus*.

Keywords: Seaweed, drying method, extraction; carrageenan; and *Kappaphycus striatus*

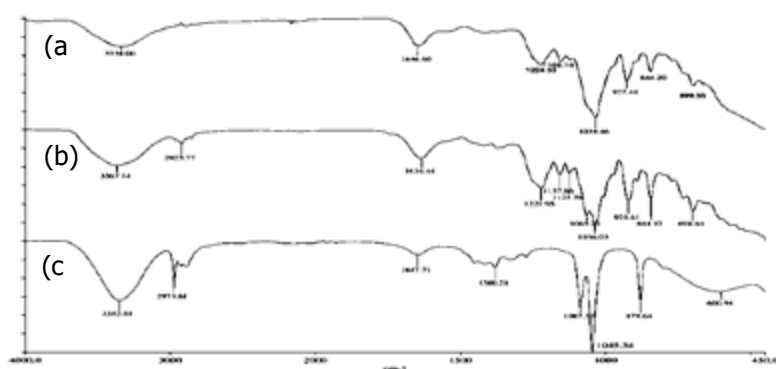


Figure 1. FTIR spectra of red *K.Striatus* for (a) Oven dried; (b) Oven dried and Hot-Water Extraction; and (c) Oven dried and Ultrasound-Assisted Extraction.

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PLASMA SURFACE MODIFICATION OF ALUMINIUM POWDER FOR GREEN HYDROGEN GENERATION

Keun Su Kim^{a,*}, Florin Saceleanu^{b,*}, Mac Parker^b, Dean Ruth^a, Mark Plunkett, Oltion Kodra, Reza Kholghy^{b,*}

^aQuantum and Nanotechnologies Research Centre, National Research Council Canada, Canada.

^bEnergy and Particle Technology Laboratory, Carleton University, Ottawa, Canada

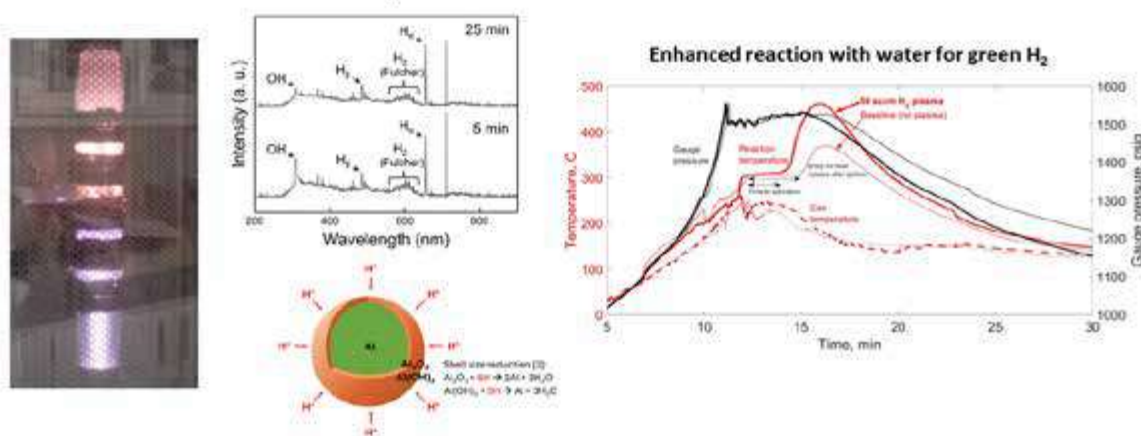
*Corresponding author: KeunSuKim@nrc-cnrc.gc.ca; florinsaceleanu@cunet.carleton.ca; RezaKholghy@cunet.carleton.ca

Abstract

For the accelerated transition towards low-carbon economy, metal powders are emerging as carbon-free energy carriers. They can turn into metal oxides in a CO₂-free environment via metal-water reaction releasing heat and hydrogen. Among various metals, aluminum is highly promising;¹ however aluminum powder contains native surface oxide layers which lead to poor reaction kinetics with water. Such oxides usually exhibit extraordinarily high thermal stability and chemical resistance rendering their effective removal extremely challenging. In this work, we developed a low-carbon footprint process for surface modification of aluminum powders using a non-equilibrium plasma (NEP).² Micron-sized (45 μm) aluminum powders were treated in both Ar and H₂ NEPs (150 W, 2~3 torr, 13.56 MHz) with different flow rates of 5, 20 and 50 sccm H₂ and 50 sccm Ar for 30 min. To assess their reactivities, the plasma-treated powders were ignited in compressed liquid water in a stainless-steel batch reactor, initially pressurized to 1,000 psig with back pressure regulation of 1,500 psig. All the H₂ plasma-treated powders reached peak temperatures 50-100 °C higher and slightly higher hydrogen yields than those of the untreated baseline and the Ar plasma. The ignition delays and the rate of heat release were also improved compare to the non-treated powders. Optical emission spectroscopy (OES) measurements during the plasma treatment confirmed the existence of both OH and H radicals in the H₂ plasma. UV-vis measurements suggest conversion of Al₂O₃ or Al(OH)₃ into AlO(OH) which is more reactive with water. Potential reaction mechanism of the native oxide layers with OH and H radicals in H₂ plasmas will be discussed.

Keywords: Green hydrogen, metal powder combustion, plasma, surface modification

Plasma surface modification of Al powder



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BARIUM–ORGANIC FRAMEWORK FOR CAPTURE AND CHEMICAL FIXATION OF CO₂ VIA CYCLIC CARBONATES AND OXAZOLIDINONES

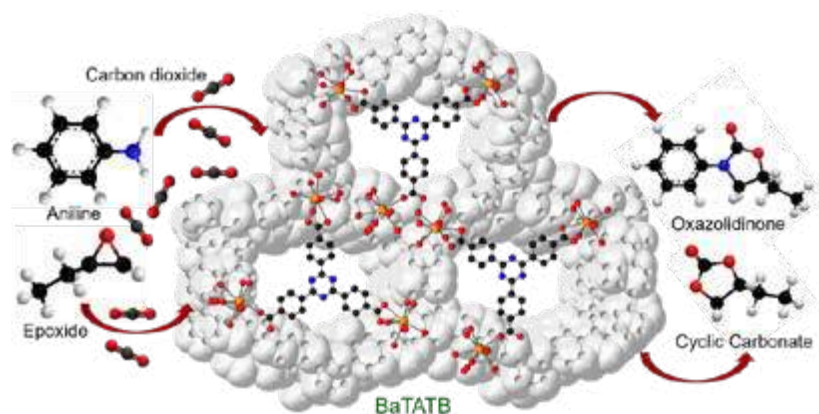
Aasif Helal

Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia
Corresponding authors: aasifh@kfupm.edu.sa (A. Helal)

Abstract

The carbon dioxide (CO₂) capture and utilization strategy has emerged as an innovative and multifaceted approach to counteract carbon emissions. In this study, a highly porous muffin polyhedral barium (Ba)–organic framework (BaTATB; H₃TATB = 4,4',4''-s-triazine-2,4,6-triyl-tribenzoic acid) was synthesized solvothermally. The three-dimensional honeycomb pore architectures were densely populated with Lewis acidic Ba(II) metal sites and basic nitrogen-rich triazines. BaTATB demonstrated selective CO₂ adsorption with high heat of adsorption. Its abundance of Lewis acidic (Ba clusters) and basic (triazine) sites makes BaTATB an ideal catalyst for the cycloaddition of CO₂ to epoxides in two- and three-component reactions. Furthermore, BaTATB is an exceptional recyclable catalyst for CO₂ cycloaddition to epoxides and aromatic amines, enabling the high-yield synthesis of cyclic carbonates and oxazolidinone at 1 bar of CO₂ under moderate, solvent-free, and cocatalyst-free conditions. Additionally, BaTATB was recycled for nine and seven consecutive cycles of cyclic carbonate and oxazolidinone synthesis with no substantial decrease in catalytic activity. Using density functional theory, we demonstrated the rational design of polyhedral metal-organic frameworks with Lewis acidic and basic sites that exhibit excellent cocatalyst-free CO₂ conversion.

Keywords: carbon dioxide, MOF, barium, cocatalyst, cyclic carbonates, oxazolidinone.



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REMOVAL OF SIX HEAVY METAL IONS FROM WATER USING A BIOCHAR-POLYANILINE COMPOSITE DERIVED FROM OIL PALM EMPTY FRUIT BUNCHES

Ravi Varma Sudaya¹, Sook-Wai Phang¹ and Kian Wei Chong¹

¹Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology (TARUMT), Jalan Genting Klang, Setapak, 53300 Kuala Lumpur, Malaysia

*Corresponding author: ravivs-wp19@student.tarc.edu.my

Abstract

Water pollution, especially due to heavy metals, is a major environmental and health concern. This study investigates a Biochar/Polyaniline composite, derived from oil palm empty fruit bunches via pyrolysis, for its ability to remove heavy metal ions from wastewater. Polyaniline was synthesized using an in-situ chemical oxidation method. The composite's efficiency was tested on nickel (II), cadmium (II), chromium (III), zinc (II), lead (II), and copper (II). FT-IR analysis identified hydroxyl, carbonyl, alkane, and alkene groups in Biochar (BC), while amine, aromatic, and alkane groups were present in Polyaniline (PANI) and the composite. UV-Vis analysis confirmed PANI's emeraldine salt state, and SEM images showed that the composite's pore sizes were similar to pure BC, enhancing thermal stability. The composite's electrical conductivity ($8.0 \times 10^{-1} - 5.6 \text{ Scm}^{-1}$) was slightly lower than pure PANI ($6.0 - 8.0 \text{ Scm}^{-1}$). Nickel (II) removal was highest, with a 75.33% removal rate. Optimization studies identified the best conditions for maximum nickel (II) removal (92.78%) at an adsorbent weight of 0.75 g, a contact time of 30 minutes, a metal concentration of 50 ppm, and pH 5. The Langmuir model fit the adsorption data best, with a maximum adsorption capacity of 8.65 mg/g. These findings highlight that the Biochar/Polyaniline composite is a cost-effective and efficient material for removing heavy metals, especially nickel (II), from wastewater, offering potential for large-scale pollution remediation.

Keywords: biochar, polyaniline, composites, adsorption, heavy metal removal

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NILE TILAPIA REVEAL MICROPLASTIC CONTAMINATION IN THE RIVER NILE IN KHARTOUM, SUDAN

Dalia Saad^{a,b,*} and Hadeel Alamin^b

Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Pretoria, South Africa.

^b School of Chemistry, Faculty of Science, University of the Witwatersrand, Johannesburg, South Africa.

**Corresponding author: dalia.saad@up.ac.za; dalia.saad@wits.ac.za*

Abstract

In recent years, microplastics have been found in the water, soil, and biota of some of the world's major rivers, including the Thames (UK), the Rhine (Germany), and the Seine (France) in Europe, the Yangtze (China), and the Amazon (South America). A notable river not on this list is probably the most famous one, the River Nile. This study aimed to investigate the occurrence, characteristics, and sources of microplastics in the River Nile in Sudan using Nile Tilapia (*Oreochromis niloticus*) as a bio-indicator. Known as Bulti in the Sudanese Arabic dialect, Nile Tilapia is an economically and ecologically dominant species in Sudan and is widely consumed. Therefore, it is a suitable target organism to bio-monitor MPs in the region. The fish samples were processed by digestion (to remove organic matter) and density separation (to extract microplastics based on their densities). Physical identification was performed using a light microscope and scanning electron microscopy (SEM), while chemical analysis was conducted using Raman spectroscopy. Microplastics were 100% prevalent. A total of 567 MP particles were recovered from the digestive tracts of the fish, with an average intensity of 18.90 ± 9.17 particles/fish and an average abundance of 72.02 ± 62.06 particles/kg. Smaller, fibrous, and coloured MPs were the most abundant size, shape, and colour, accounting for 84%, 85%, and 84%, respectively. This likely reflects a higher abundance of small-sized microplastics in the river, resulting from frequent fragmentation through various environmental processes. Furthermore, small-sized MPs have a larger surface area, which facilitates biofouling and the attachment of other contaminants, reducing their buoyancy and increasing their bioavailability. Polypropylene (PP) and high-density polyethylene (HDPE) were the two polymers identified in the samples, indicating their widespread usage and persistence in the environment. This scoping study provided the first data on microplastic contamination in the River Nile in Sudan.

Keywords: Microplastics, bio-indicator, River Nile, Nile Tilapia, Sudan.

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INTEGRATING EXPERIMENTAL AND COMPUTATIONAL TOOLS FOR ADSORPTIVE REMOVAL OF DICAMBA USING UiO-66(ZR)-IMPREGNATED CHOLINIUM ALANATE IONIC LIQUID

Norlaylawate Mohd Kama¹, Noor Fazriyana Hamidon¹, Hayati Mukhair¹, Erma Fatiha Muhammad¹, Hayyiratul Fatimah Mohd Zaid², Yeek Chia Ho³, Nur Nadhirah Mohamad Zain⁴, Marzhan S. Kalmakhanova⁵ and Khairulazhar Jumbri^{1,*}

¹ Department of Fundamental and Applied Sciences, Center of Research in Ionic Liquids (CORIL), Institute of Sustainable Energy and Resources (ISER), Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia.

² Department of Chemical Engineering, Centre of Innovative Nanostructure and Nanodevices (COINN), Institute of Smart and Sustainable Living, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia.

³ Department of Civil and Environmental Engineering, Centre for Urban Resource Sustainability, Institute of Smart and Sustainable Living, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia

⁴ Department of Toxicology, Advanced Medical and Dental Institute, Universiti Sains Malaysia, Bertam, 13200 Kepala Batas, Penang, Malaysia.

⁵ Department of Chemistry and Chemical Technology, M.Kh. Dulat Taraz University, Taraz 080012, Kazakhstan

*Corresponding author: khairulazhar.jumbri@utp.edu.my

Abstract

Dicamba herbicide contamination in water sources poses significant environmental risks, necessitating effective removal strategies. This study investigates the development of hybrid adsorbents by incorporating [Ch][Ala] ionic liquid into UiO-66(Zr) metal-organic frameworks to enhance adsorption performance. The hybrid materials were synthesized and characterized using NMR, XRD, FESEM, BET, FTIR, and TGA, confirming structural stability and successful incorporation of [Ch][Ala]. Adsorption experiments, optimized using response surface methodology (RSM) and machine learning, demonstrated that the 5% [Ch][Ala]-loaded hybrid achieved a maximum Dicamba removal efficiency of 99.51%. The adsorption followed the pseudo-second-order model, indicating the chemisorption is the primary control mechanism in the adsorption process. Isotherm studies revealed that the adsorption data fit well with the Langmuir isotherm model, indicating monolayer adsorption on homogeneous surfaces with the maximum adsorption capacities of 72.31 and 78.02 mg/g for pristine and UiO-66(Zr)/[Ch][Ala]@5%, respectively. The adsorption thermodynamics confirmed the feasibility of the reaction and spontaneity of the adsorption process. The enhancement in adsorption capacity of Dicamba can be attributed to functional groups introduced by [Ch][Ala], through π - π and hydrogen bonding which enhance interactions between the adsorbate and hybrid MOF adsorbent.

Keywords: Adsorption; UiO-66(Zr), dicamba; machine learning; kinetics; isotherms; docking.

CORROSION INHIBITION SCREENING OF NITROBENZALDEHYDE MELDRUM'S ACID USING RESPONSE SURFACE METHOD AND MACHINE LEARNING

Muhammad Azhan Arif Mansor^a, Sheikh Ahmad Izaddin Sheikh Mohd Ghazali^a, Nurul Auni Zainal Abidin^a, Tuan Norhafizah Tuan Zakaria^b, Nur Nadia Dzulkifli^{a*},

^a*School of Chemistry and Environment, Faculty of Applied Sciences, Universiti Teknologi MARA Cawangan Negeri Sembilan, Kampus Kuala Pilah*

^b*College of Computing, Informatics and Mathematics, Universiti Teknologi MARA Cawangan Negeri Sembilan, Kampus Kuala Pilah*

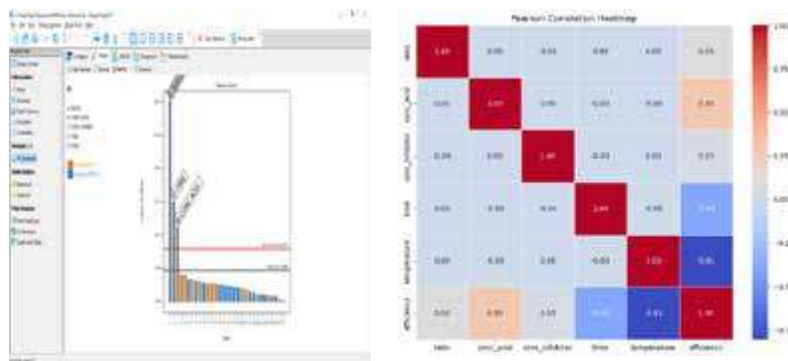
**Corresponding author: nurnadia@uitm.edu.my*

Abstract

Corrosion inhibitors are substances that, when added in small quantities to an acidic environment, reduce the rate of corrosion. Thus, the objective study is to screen and evaluate the corrosion inhibition of nitrobenzaldehyde Meldrum's Acid (NBMA) in HCl medium. The NBMA compound was successfully synthesized through a condensation method and characterized using elemental analysis, ATR-FTIR and NMR spectroscopies. Weight loss measures revealed that the corrosion inhibition efficiency of NBMA increases with its concentration. The adsorption of NBMA onto mild steel surfaces adhered to the Langmuir isotherm, with an R^2 value of 0.999, indicating the formation of a monolayer on the mild steel surface, as further confirmed by SEM-EDX analysis. The Gibbs Free Energy value of -25.011 kJ/mol suggests that the adsorption process involves both physisorption and chemisorption mechanisms. Following this, NBMA will be screened using Response Surface Methodology (RSM) with two factors, incorporating temperature, acid concentration, inhibitor concentration, time, and ratio as parameters. The results indicated that temperature, time, and acid concentration significantly influence the inhibition efficiency. These findings are further supported by computational analysis using the Pearson model, which revealed that temperature, acid concentration, and time are the most strongly correlated parameters with inhibition efficiency.

Keywords: RSM, Machine Learning, Meldrum's Acid, Corrosion, Langmuir isotherm

Graphic / Image



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CONTROLLABLE INTRODUCTION OF EDGED NITROGEN SITES IN CVD-DERIVED CARBON MATERIALS FOR ENHANCED FENTON-LIKE REACTIONS

Ying Chen*

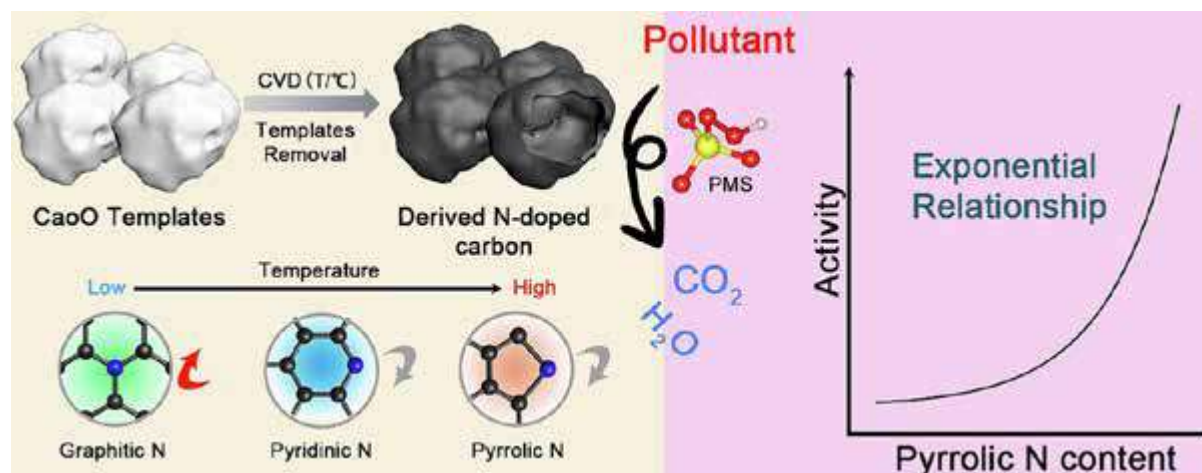
Department of Chemical Engineering, Tianjin Renai College, Tianjin 301636, China

*Corresponding author: yingchen@tju.edu.cn

Abstract

Nitrogen doped carbon materials have great potential in the peroxymonosulfate (PMS) based advanced oxidation processes due to their high efficiency.¹ However, because of the limitation of prepared method, the doped N species are usually uncontrollable. In this work, a series of metal-free N-doped carbon materials are synthesized by chemical vapor deposition (CVD) with CaO as the template and pyridine as the deposition precursor. Through regulating the deposition temperature, we achieve the gradient control of the edged-N species.² Taken phenol as the pollutant probe, the catalytic performances of N-doped carbon material are investigated with PMS as the oxidant, and 700 °C is determined to be the optimal deposition temperature for carbon material with a reaction rate constant of 0.335 min⁻¹. The N species are analyzed by XPS spectra for the samples obtained from different temperature. After the analysis of kinetics and the N species, we demonstrate that the content of pyrrolic N has an exponential relationship with the activity. Radicals quenching experiments, electron paramagnetic resonance and electrochemical test are also employed to verify that O₂^{•-}, ¹O², and direct electron transfer are the dominated reactive oxidation species rather than typical hydroxyl and sulfate radicals.³ Overall, this doped strategy through CVD give a new insight of controlling doped species in carbon materials preparation.⁴

Keywords: CVD-derived carbon, Edged nitrogen sites control, Fenton-like reaction activity, Exponential relationship



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SUSTAINABLE DUCKWEED DERIVED ADSORBENTS FOR WASTE WATER TREATMENT

Alvin Lim Teik Zheng^{a,b*}, Ellie Teo Yi Lih^b, Sivasanger Seenivasagam^{a,b}, Yiu Pang Hung^b

^a Institute of Ecoscience Borneo, Universiti Putra Malaysia Bintulu Sarawak Campus, Bintulu 97008, Sarawak, Malaysia

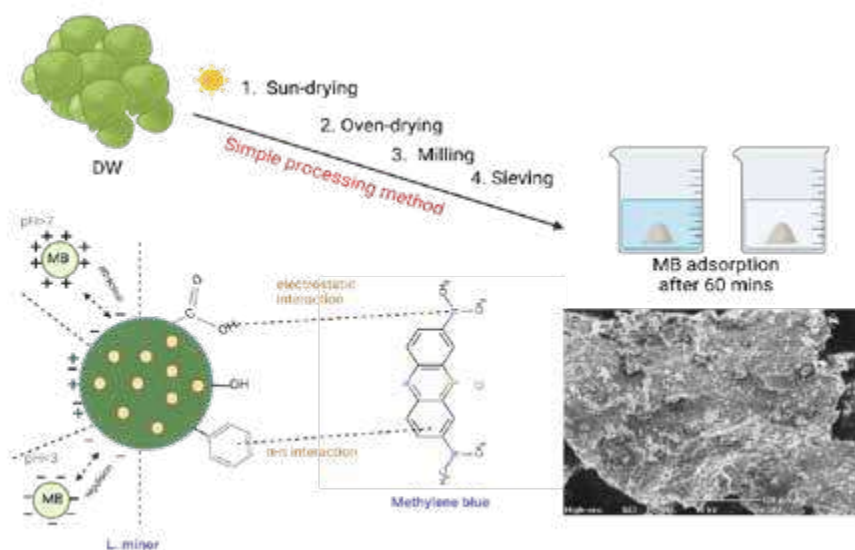
^b Department of Science and Technology, Faculty of Humanities, Management and Science, Universiti Putra Malaysia Bintulu Sarawak Campus, Bintulu 97008, Sarawak, Malaysia

*Corresponding author: alvintz@upm.edu.my

Abstract

Invasive plants threaten natural ecosystems due to their rapid spread and growth. This study used a duckweed (DW) plant to develop a low-cost and sustainable adsorbent to remove methylene blue (MB) from aqueous solution. Fourier transform infrared spectroscopy (FT-IR) identified oxygen-containing functional groups on the DW surface that enhanced its adsorption capacity. Optimal adsorption conditions were achieved with an adsorbent amount of 20 mg, a pH of 10, and an initial MB concentration of 10 mg/L. Experimental data matched the pseudo-second-order (PSO) model across all concentrations, including 10 mg/L ($Q_e = 73.53$ mg/g), 20 mg/L ($Q_e = 183.15$ mg/g), and 50 mg/L ($Q_e = 200.80$ mg/g). The Temkin isotherm model fit the data better than the Langmuir and Freundlich models. Adsorption decreased with increasing temperatures ($\Delta G^\circ = -7.56$ to -8.06 kJ/mol, $\Delta H^\circ = -4.93$ kJ/mol, $\Delta S^\circ = -6.76$ kJ/mol). The primary adsorption mechanisms included electrostatic interactions, hydrogen bonding, and π - π electron interactions. The production cost of the DW adsorbent was estimated at RM 14.40 per kg, indicating its potential as a cost-effective option. With its high adsorption capacity and wide availability, DW is a promising material for controlling dye pollution in wastewater.

Keywords: duckweed, adsorption, methylene blue, sustainable



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COMPARATIVE GREEN PRACTICES TO EXTRACT AND CHARACTERIZE THE DIFFERENT PRECIOUS, TOXIC AND RARE EARTH METALS FROM E-WASTES

Giri J^{a,b,*}, Aryal G^a, Joshi HR^a, Adhikari M^a, Rakesh Das^c, Henning S^d, Adhikari R^e

^aTri-Chandra Multiple Campus, Tribhuvan University, Ghantaghar, Kathmandu Nepal.

^bNepal Polymer Institute, Kathmandu, Nepal.

^cDepartment of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, India.

^dFraunhofer Institute for Microstructure of Materials and Systems (IMWS), Halle, Germany.

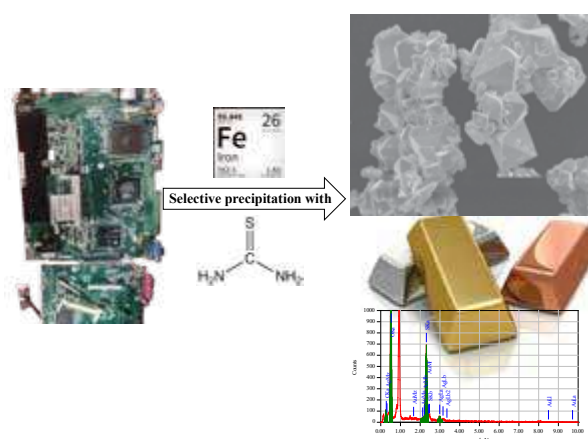
^eResearch Centre for Applied Science and Technology, Tribhuvan University, Kirtipur, Nepal.

*Corresponding author: girijys@yahoo.com

Abstract

Electrical and electronic gadgets (E-gadgets) contain various elements for specific smart applications. These metals after the dead use of E-gadgets discarded from circular economy and become electrical and electronic waste (E-waste). The huge production of E-waste has become headache of the world. This work tries to explore the methods to extract various precious (gold, silver, copper), toxic (lead), and rare earth metals (Yttrium) from different E-waste such as printed circuit board (PCB), lead acid battery, LCD and LED display monitor and study their properties for reuses. Hydrometallurgy and selective precipitation with green solvents such as dilute H_2SO_4 , thiourea, dilute NaOH and methylene sulphonic acid (MSA) were one among the best techniques applied in this work. The extracts were characterized to illustrate their purity, constituents, state and structure by different techniques such as fourier transform infrared spectroscopy (FTIR), optical microscopy (OM), UV-visible spectroscopy (UV-vis), energy dispersive X-ray (EDX) and scanning electron microscopy (SEM) etc. The result reveals the metallic and combined oxide states are as pure as they are commercially available in the market. Copper are extracted in oxide state from PCB board with fcc crystal system, Similarly gold and silver are extracted in thiourea complex state. The α - and β -PbO are extracted from lead acid battery, Yittrium, extracted as Y_2O_3 from CRT and LCD monitor using comparatively environmentally friendly reagents

Keywords: E-waste, hydrometallurgy, energy dispersive X-ray (EDX), scanning electron microscopy (SEM), selective precipitation



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PHOTODEGRADATION PATHWAY OF BISPHENOL S BY TITANIUM DIOXIDE UNDER UVA IRRADIATION

Sharon Fatinathan^{a,*}, Siti Nur Hajar Mohamed Anuar^a, Tavamani Balan^a
and Vikneswari Perumal^b

^a*Faculty of Pharmacy and Health Sciences, Royal College of Medicine Perak, Universiti Kuala Lumpur,
30450 Ipoh, Perak, Malaysia*

^b*School of Pharmacy, Management and Science University, University Drive, Off Persiaran Olahraga,
40100 Shah Alam, Malaysia*

*Corresponding author: sharon@unikl.edu.my

Abstract

Plastic pollution has emerged as a significant global challenge in recent years. It is estimated that 5-10% of the worldwide plastic production ends up in the oceans annually¹. In 2020, Malaysia's plastic consumption amounted to 148 thousand metric tons, with an annual per capita of 16.78 kg². The "Malaysia Roadmap Towards Zero Single-Use Plastics 2018-2030" was introduced as a three-phase national plan to eliminate single-use plastics³. However, existing plastic waste can snowball into an environmental crisis, as plastic and microplastic waste release various additives during fragmentation. Among these additives, Bisphenol S (BPS) has been identified as an emerging pollutant with the potential to adversely affect humans and animals. Therefore, the removal of this analog from wastewater is essential. This study evaluated the effectiveness of titanium dioxide (TiO₂) in photodegrading BPS in an aqueous solution under UVA light while elucidating the photodegradation pathways. Key photodegradation parameters, including the initial pH of the solution, photocatalyst dosage, and illumination period, were optimized. UV-visible spectrophotometer results showed that at an initial concentration of 5 mg/mL, complete photodegradation of BPS occurred within 180 minutes under UVA exposure. Kinetic study showed that the photodegradation process followed the Langmuir-Hinshelwood kinetic model, with a rate constant of 0.0133 min⁻¹. High-performance liquid chromatography (HPLC) analysis identified a single intermediate persisting in the solution after 180 minutes of photodegradation. However, liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis detected four distinct photodegradation peaks and elucidated their formation pathways, revealing a complex degradation pathway. Overall, this study provides valuable insights into the photocatalytic degradation of BPS using TiO₂ under UVA irradiation. HPLC and LC-MS/MS analyses confirmed that while BPS undergoes significant degradation under UVA light in the presence of TiO₂, its degradation products persist as intermediate in the solution.

Keywords: titanium dioxide; bisphenol S; photodegradation; UVA; pathway

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THE EFFECTS OF SUPPLEMENTARY MATERIALS ON MECHANICAL PROPERTIES OF ORDINARY PORTLAND CEMENT WITH LOW-LIME CALCIUM SILICATE POWDER

G.M. Kim^{a,b,*}, Jemal Kedir Adem^{a,b}

^a*Mineral Processing & Metallurgy Research Center, Resources Utilization Division, Korea Institute of Geoscience and Mineral Resources, 124 Gwahak-ro, Yuseong-gu, Daejeon 34132, Republic of Korea.*

^b*Department of Resources Recycling, University of Science and Technology, 217 Gajeong-ro, Yuseong-gu, Daejeon 34113, Korea*

**Corresponding author: k.gm@kigam.re.kr*

Abstract

Carbon dioxide emissions from the cement industry account for approximately 8% of total industrial emissions. Low-lime calcium silicate cements are one of the promising alternatives to Ordinary Portland cement. The use of low-lime calcium silicate cement could potentially reduce the CO₂ emission by up to 40% compared to Ordinary Portland cement. The incorporation of supplementary materials such as blast furnace slag and fly ash possibly contributes to a further reduction in the CO₂ emission of cement industry. However, the relevant studies on the combined effects of low-lime silicate powder and supplementary materials have been rarely conducted. The effects of supplementary materials on mechanical properties of Ordinary Portland cement with low-lime calcium silicate powder in the present study were investigated via compressive strength, thermogravimetric mercury intrusion porosimetry tests so on. The detailed the results will be present.

Keywords: low-lime calcium silicate cement; carbon dioxide; ordinary Portland cement; supplementary materials.

Acknowledgment

This work was supported by the industrial strategic technology development program-development of manufacturing technology of hardened cement with carbonation curing (RS-2022-00155662, Development of manufacturing and application technology of 1,000 ton/year class hardened cement with carbonation curing) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea).

BIO-ADSORBENT TOWARD POTENTIAL REMEDIATION OF HIGHLY POLLUTED BAGMATI RIVER WATER, KATHMANDU, NEPAL

Mandira Pradhananga Adhikari*

Central Department of Chemistry, Tribhuvan University, Kathmandu, Nepal

**Corresponding author: mandira43@hotmail.com*

ORCID: 0000-0002-5183-8343

Abstract

The water quality of the geographically and culturally precious Bagmati River is deteriorating continuously due to the mixing of industrial and municipal waste and highly polluted tributaries. To overcome the uncertainties of the traditional water quality monitoring system, a sophisticated real-time mobile-sensor system, the first experience of a river water monitoring system in Nepal, was incorporated, which provides fine-scale large data sets of water quality parameters. The physicochemical parameters were measured on the spot, and chemical and biological parameters were determined in the laboratory. The results indicated that the pollutants in the Bagmati River water increased and decreased oxidation-reduction potentials (ORP) and dissolved oxygen (DO), converting a hypoxic state downstream inside the Kathmandu Valley¹. The total coli form count was extremely high, and the bacterial count exceeded the limit even in a 10-fold diluted sample, attributing the faecal pollution¹. The discharge of domestic effluent, the disposal of solid waste along the bank of the river, and the mixing of highly polluted tributaries turned the Bagmati River into a biologically dead river downstream². Such polluted river water was successively treated with the nanoporous-activated carbons and *Moringa oleifera* seed extract. After treatment, the black water was turned into clear and clean water with the potential reduction of pollutants (>80%) and coliform and bacterial counts to the WHO-recommended values³.

Keywords: Activated carbon, *Moringa oleifera*, ORP, water pollution.

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GASIFICATION OF SOLID WASTE FOR HIGH-PURITY H₂ PRODUCTION WITH NEGATIVE CO₂ EMISSIONS

Xiuping Liao^a, Soo Jean Park^b, Yijiao Jiang^{a,*}

^a*School of Engineering, Macquarie university*

^b*Applied BioScience, Macquarie University*

*Corresponding author: yijiao.jiang@mq.edu.au

Abstract

Gasification of solid waste offers a cost-effective approach to producing hydrogen (H₂)¹, a crucial energy carrier for the future low-emission energy system². However, the conventional steam gasification approach demands substantial energy and freshwater inputs for pre-drying waste feedstock and generating steam, while also generating carbon dioxide (CO₂) emissions.^{3,4} To address these challenges, this study first explored the feasibility of directly using the initial moisture of biosolids as an in-situ steam source for H₂ production in a two-stage process with the presence of calcium oxide (CaO) as the CO₂ sorbent. In the second stage, different amounts of CO₂ were introduced to investigate its potential to convert more carbon into carbon monoxide (CO). Results showed that the in-situ generated steam successfully enhanced H₂ yield and improved H₂ purity in the first stage, which was comparable to the H₂ production in conventional steam process. By incorporating CO₂ gasification of char in the second stage, the CO yield was increased by 1.2 times, through enhancing the reverse Boudouard reaction between CO₂ and residue solid carbon. As a result, negative net CO₂ emission was achieved with up to 3.8 kg of CO₂ being eliminated for producing one kilogram of H₂. Moreover, a techno-economic analysis demonstrated that the levelized cost of hydrogen (LCOH) can be reduced to 2.0 US\$/kg when the plant capacity is over 1220 kg/h. This study presents an efficient approach to harnessing hydrogen from solid waste with low cost and low emissions.

Keywords: Waste gasification, biosolids, hydrogen, CO₂ emission

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FOAM FRACTIONATION FOR REMEDIATION OF PFAS: EFFECT OF PHYSICOCHEMICAL PROPERTIES

Reza Foudazi^{a,*}, Muchu Zhou^a

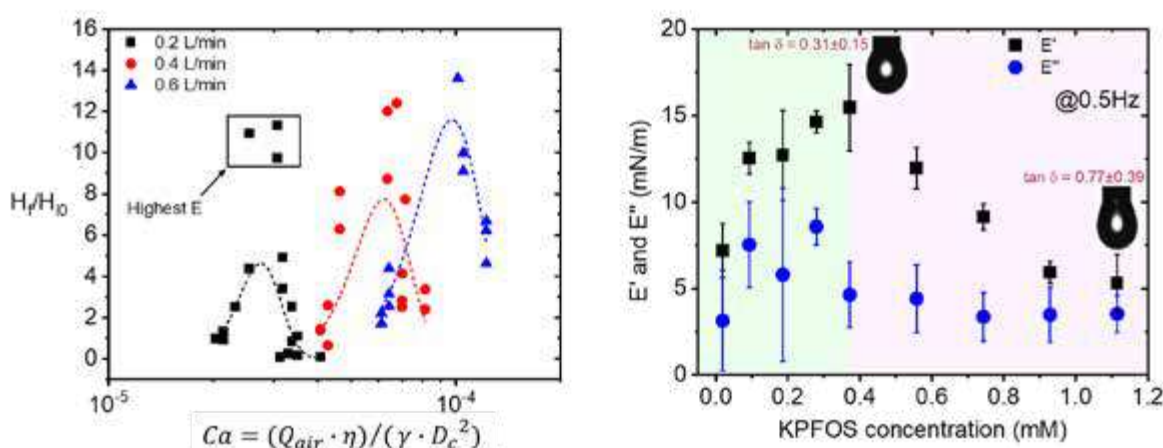
^a School of Sustainable Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, OK 73019, USA.

*Corresponding author: rfoudazi@ou.edu

Abstract

Per- and polyfluoroalkyl substances (PFAS) are a diverse group of partially or fully fluorinated manmade organic compounds, which have been applied into numerous applications, such as nonstick cookware and aqueous film-forming foams (AFFFs). While the PFAS offer significant benefits, their propensity to accumulate in living organisms and environment, particularly water bodies, raises substantial health concerns. Foam fractionation, a method targeting surfactants and colloids, holds promise for removing PFAS from water; however, its current employment in PFAS removal is limited. Moreover, the correlation between the interfacial properties of PFAS and their foaming behavior has not been extensively studied or methodically examined. Therefore, a profound understanding of the air-water interfacial properties of PFAS is key to improving the practicality of employing foam fractionation for the removal of PFAS from polluted water sources going forward. This presenting work studies the foaming characteristics of PFAS, revealing that PFAS with longer chains display better foam formation and foam stability. Dimensional analysis is used to correlate the foaming behavior of PFAS to several dimensionless parameters. Additionally, this study investigates how the addition of electrolytes affects both the interfacial properties of PFAS and their behavior in forming foam.

Keywords: Adsorption, Interface, Langmuir isotherm, Interfacial rheology, Bubble size.



ELECTROCHEMICAL CHARACTERIZATION OF COCONUT SHELL DERIVED ACTIVATED CARBON FOR SUPERCAPACITOR APPLICATION

Armila Rajbhandari (Nyachhyon)^{a*}, Sarmila Dangi^b, Sharmila Pradhan (Amatya)^b,
Santosh Khanal^a

^aCentral Department of Chemistry, Tribhuvan University, Kirtipur, Nepal

^bAscol Campus, Tribhuvan University, Lainchour, Nepal

*Corresponding author: armila.rajbhandari@cdc.tu.edu.np

Abstract

Coconut shell derived activated carbon was successfully prepared by phosphoric acid activation followed by carbonization at 400°C for 3 hours in an inert nitrogen atmosphere. Thus prepared activated carbon was characterized by Scanning Electron Microscopy (SEM), X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Methylene Blue (MB_N) and Iodine number (I_N). Results revealed that as prepared material was found to be amorphous having oxygenated surface functional groups with the specific surface area 802.12 m²g⁻¹ (±0.59%). MB_N and I_N was found to be 181.52 mg g⁻¹ and 821.7 mg g⁻¹ respectively indicating the presence of mesopores and micropores. Electrochemical characterization was also performed by three-electrode system where carbon electrode was used as working electrode, platinum plate was used as counter electrode and Ag/AgCl electrode was used as a reference electrode. The experiments were performed in 2 M aqueous KOH using Cyclic Voltammetry (CV), Galvanostatic Charge–Discharge (GCD) and Impedance Spectroscopy (EIS). The specific capacitance acquired from GCD at 1 Ag⁻¹ was found to be 136.4 Fg⁻¹ (±0.13%) with 2.1 Ω (±0.3%) ESR. Results are in good agreement with literature value¹⁻³. The energy density and power density of carbon electrode was found to be 68.21(±0.25%) W h kg⁻¹ and 600 (±0.5%) W kg⁻¹ respectively⁴. The results exhibited that the desirable electrochemical capacitive performances enable the coconut shell derived activated carbon to act as a bio material for high-performance supercapacitors and energy storage devices.

Keywords: Activated carbon, Coconut shell, Phosphoric acid Activation, Electrochemical characterization, Supercapacitor

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CARBON DIOXIDE CATALYTIC CONVERSION INTO VALUABLE PRODUCTS: A SUSTAINABLE APPROACH

L. C. Branco*, V. Paz, S. Messias, A. I. Paninho, C. I. Melo, A. R. Machado, A. V. Nunes

LAQV-REQUIMTE, NOVA School of Science and Technology, 2829-516 Caparica, Portugal

* E-mail: l.branco@fct.unl.pt Abstract

Abstract

The emergence of carbon dioxide (CO₂) methanation as a promising strategy for mitigating greenhouse gas emissions and advancing carbon capture and utilization (CCU) represents a significant step in addressing global climate challenges. This process not only reduces CO₂ emissions but also facilitates the production of renewable energy by converting carbon dioxide into methane, offering a viable pathway toward carbon neutrality [1].

Through CO₂ hydrogenation, a diverse range of valuable chemicals can be synthesized, including formic acid, formate, methane, lower olefins, higher hydrocarbons, methanol, and higher alcohols—many of which serve as fuels. However, a key challenge in CO₂ conversion lies in the inherent stability of the molecule, which requires substantial energy for activation. A promising solution involves a biphasic system consisting of excess CO in the gas phase and an imidazolium-based ionic liquid (IL) in the stationary phase. This approach enables CO₂ methanation under relatively mild conditions. The unique properties of ILs promote the formation and stabilization of highly active ruthenium nanoparticles, which effectively catalyze the reaction, achieving an optimized methane yield of 84% at 150°C [2, 3]. Recent research has explored innovative methods to enhance the efficiency and sustainability of this reaction, including the use of deep eutectic solvents as alternative media and covalent organic frameworks (COFs) as porous catalytic supports. Some of these catalytic strategies are being developed for continuous processes in collaboration with industrial partners. Additionally, alternative CO₂ catalytic approaches are under investigation, such as the electroreduction of CO₂ to syngas in aqueous IL media [4] and the synthesis of cyclic carbonates through homogeneous or heterogeneous catalysis in IL-based systems [5]. These advancements mark significant progress toward more efficient and sustainable CO₂ utilization methods, which could play a crucial role in combating climate change and accelerating the transition to a low-carbon economy.

Keywords: CO₂ valorization; Ionic Liquids&Eutectic Systems; Covalent Organic Frameworks; Methane; Cyclic Carbonates

Acknowledgements

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EVALUATIONS OF BIOBED SYSTEMS PROCESSING PESTICIDE RINSATE - THE CANADIAN PRAIRIES PERSPECTIVE

Annemieke Farenhorst^{a*}, Phoenix Nakagawa^a, Ifeoluwa F. Omotade^b, Kayla Talabis^a, Marufa Fatema^a, Ruwani Wimalasekara^c, Alistair Brown^a, Ayush Kumar^c, Ramanathan Sri Ranjan^b, Sarah Johnson^a

^a*Department of Soil Science, University of Manitoba, Winnipeg, MB, Canada.*

^b*Department of Biosystems Engineering, University of Manitoba, Winnipeg, MB, Canada.*

^c*Department of Microbiology, University of Manitoba, Winnipeg, MB, Canada.*

^{*}*Corresponding author: annemieke.farenhorst@umanitoba.ca*

Abstract

Biobeds are used throughout the world as a best management practice in recycling pesticide rinsate. Focusing on pest control products used in grain and oilseed production in the Canadian Prairies, this research validated analytical methods (Eurachem guidelines) to quantify 80+ pesticide active ingredient in matrices such as pesticide rinsate, biomatrix, and biobed effluents. Analytes included glyphosate, the most popular herbicide worldwide, and its primary metabolite AMPA, as well as herbicides 2,4-D, atrazine, dicamba and clopyralid. The research also applied DNA extractions and 16S sequencing to assess the relative abundance of bacterial phyla in biomatrix. Data were collected from a dual cell biobed system that processed up to ~10,000 L pesticide rinsate per year. The first cell receives direct rinsate and so larger pesticide concentrations, than the second cell which receives the effluent from cell one. Data showed that the biobed was highly efficient, and that there was a clear need for a second cell to process pesticide rinsate into cleaner water. Data from other dual- and single-cell biobeds in the Canadian Prairies also demonstrated an excellent biobed efficiency with biobed effluent showing a much smaller Pesticide Toxicity Index than the added pesticide rinsate. Pesticides loadings into cells one or two did not appear to have a profound impact on the relative abundance of bacterial phyla in the biomatrix, in part, because of substantial spatial variations in bacterial phyla within each biobed cell. Biobeds were least effective for current-use pesticides that have groundwater ubiquity scores (GUS values) greater than 2.8; and some analytes were consistently detected in final effluent at low levels (e.g., AMPA, bentazon, clopyralid). In Canada, at least 100 million kg of pesticide active ingredients are sold annually for use in agricultural (~70%) and non-agricultural applications (~30%). This study supports the adoption of biobeds in socio-economic sectors applying pesticides.

Keywords: herbicides, biobeds, ultra-high performance liquid chromatography, liquids, semi-solids, green economy, source water protection.

TURNING WASTE INTO VALUE: INNOVATIVE APPROACH OF HYDRATED LIME WASTE FOR CO₂ CAPTURE

Shazleen Saadon^{a*}, Safwan A. Salam^b

PETRONAS Research Sdn Bhd

*Corresponding author: shazleen.saadon@petronas.com

Abstract

Direct air capture (DAC) of CO₂ is a potential technique for reducing climate change. However, its global implementation is challenging due to high energy consumption and material costs. This study investigates the feasibility of using hydrated lime waste, a byproduct of acetylene production, as an economical and accessible sorbent material for direct air capture (DAC). The hydrated lime waste, primarily composed of calcium hydroxide (Ca(OH)₂), possesses inherent CO₂ capture capabilities. First, the material's properties were characterized for its mineralogical composition, surface area, and porosity using XRD, SEM, and BET. Next, CO₂ capture experiments are conducted in a controlled environment to assess the sorption capacity and kinetics of hydrated lime waste. When hydrated lime waste is exposed to air, it reacts with CO₂ to form layers of CaCO₃, which can then be used for other purposes. As examples, usage in water treatment or for binding agent in concrete-making. The chain of chemical process demonstrates the potential of hydrated lime waste as a cost-effective and sustainable alternative to conventional DAC sorbents by valorizing industrial waste and reducing the reliance on energy-intensive materials.

Keywords: direct air capture, hydrated lime waste, carbon capture



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INNOVATIVE CUR-CPTMS-NZC BEADS FOR EFFICIENT AND SUSTAINABLE METHYLENE BLUE DYE REMOVAL FROM AQUEOUS SOLUTIONS

Mohd Ridhwan ADAM^{a,*}, Nur Fatin Atikah Abdul MUTALIB^a, Azat SEITKHAN^b,
Norliyana Mohd SALLEH^c

^aMaterials Technology Research Group (MaTReC), School of Chemical Sciences, Universiti Sains Malaysia,
11800 Minden, Penang, Malaysia.

^bLaboratory of Engineering Profile, Satbayev University, 22 Satbayev Str., Almaty, Kazakhstan.

^cAcademic Research Management, Group Technology and Commercialisation, PETRONAS Research Sdn Bhd,
43000 Bandar Baru Bangi, Selangor, Malaysia

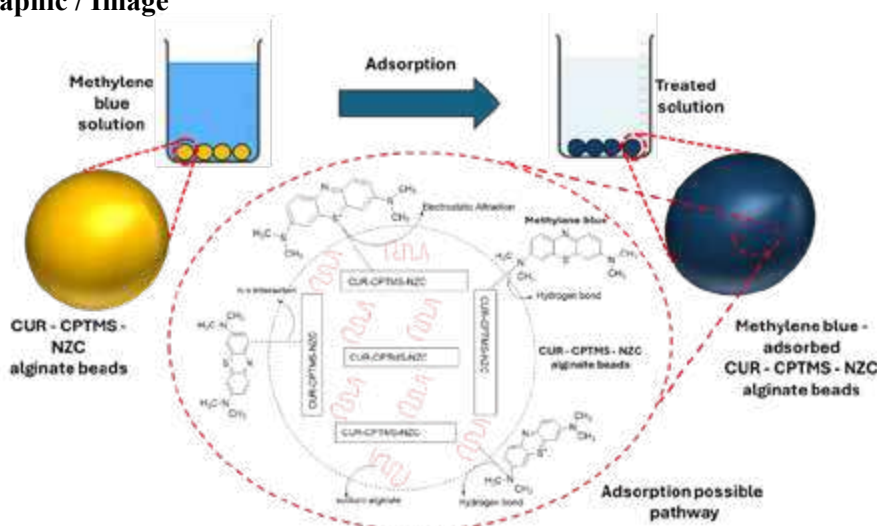
*Corresponding author: mohd.ridhwan@usm.my

Abstract

This study effectively fabricated curcumin-functionalized chloropropyl trimethoxy silane-natural zeolite clinoptilolite (CUR-CPTMS-NZC) beads by utilizing acid-pretreated natural zeolite clinoptilolite (HCl-NZC) in combination with curcumin, which were then integrated into alginate beads. These beads were engineered to effectively eliminate methylene blue (MB) dye from aqueous solutions, emphasizing environmental sustainability. A thorough characterization was conducted utilizing FTIR, BET, TGA, SEM-EDX, and zeta potential analysis. The optimization of removal efficiency was achieved by examining the impacts of pH, adsorbent dose, and beginning MB concentration utilizing Response Surface Methodology (RSM) grounded on a Central Composite Design (CCD). The results demonstrated a robust alignment with a quadratic polynomial model, as evidenced by the elevated R^2 value (0.9967). The ideal parameters for attaining complete MB removal were identified as a pH of 7.8, a CUR-CPTMS-NZC bead dosage of 0.5 g, an initial MB concentration of 13 ppm, and a contact duration of 60 minutes. The SEM-EDX examination validated MB adsorption onto the beads' surface. The Redlich-Peterson isotherm most accurately represented the adsorption data, with a pronounced inclination towards the Langmuir isotherm, indicating that monolayer adsorption is the predominant process. The beads exhibited remarkable reusability during six successive cycles, underscoring their durability, efficiency, and potential for prolonged use in dye removal applications.

Keywords: Curcumin-functionalized zeolite; Alginate beads; Wastewater treatment; Adsorption optimization; Response Surface Methodology

Graphic / Image



REPURPOSING LOCAL AGRO-WASTE: A NOVEL STRATEGY FOR IMPROVING AGRICULTURAL WATER QUALITY

Mohammad Shahid Shahrin^{a,*}, Jamaliah Jaafar^a, Norlida Mohamed Hamim^a, Ruwaida Abdul Wahid^b, Azrizal Ahmad Rashdi^a, Nabila Arshad^a and Nur Syarafana Mohd Tajuddin^a

^a*Soil Science, Water and Fertiliser Research Centre, MARDI Headquarters, 43400 Serdang, Selangor*

^b*Engineering Research Centre, MARDI Headquarters, 43400 Serdang, Selangor*

**Corresponding author: shahid@mardi.gov.my*

Abstract

The prevalent use of agrochemicals to enhance crop yield and quality has resulted in significant environmental contamination. These substances pose a considerable risk due to their ability to undergo various chemical transformations and metabolic processes, producing byproducts that are often more toxic than the original compounds. When these chemicals are applied to crops, they do not remain confined to the targeted area; instead, they disperse through the environment, settling on plants, soils, and water bodies. This dispersion leads to the spread of pollutants across different environmental compartments, which can cause long-lasting ecological impacts. Although fertilizers are primarily composed of essential nutrients such as ammonium, phosphate, and potassium, they may also contain trace amounts of other elements like boron, sodium, magnesium, and various metals, which can further complicate their environmental effects. Recent research suggests that biochar produced from local agro-waste—specifically from rice husks, bamboo, and coconut shells—can act as an efficient bio-adsorbent for these agrochemicals, thereby mitigating their adverse environmental effects. The use of locally sourced agricultural waste to produce biochar not only represents a sustainable and cost-effective solution but also offers a reliable material for large-scale environmental remediation efforts.

Keywords: Biochar, adsorbent, heavy metals, pesticide

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CHARACTERIZATION OF NONPOLAR ORGANIC POLLUTANTS IN THE AMBIENT AEROSOLS OF DHAKA MEGACITY DURING WINTERTIME

Mohammad Lokman Hossain

Department of Chemistry, Jagannath University, Dhaka-1100, Bangladesh

**Corresponding author: lokman@chem.jnu.ac.bd*

Abstract

According to the world air quality report 2024, Bangladesh is the 2nd ranked polluted country and Dhaka city is the 3rd ranked polluted city in the world.¹ Therefore, air pollution is a big concern for Bangladesh. This study examines the molecular composition of nonpolar organics such as n-alkanes, polycyclic aromatic hydrocarbons (PAHs), hopanes, and steranes in fine particulate matter (PM_{2.5}) in Dhaka, Bangladesh, during the winter of 2020. Results reveal that organic compound concentrations were higher at night (mean: 192 ng m⁻³) than during the day (mean: 87.3 ng m⁻³), likely due to atmospheric inversion layers and elevated nighttime emissions from heavy-duty vehicles. Among the detected compounds, n-alkanes were the most abundant (mean: 454 ng m⁻³), followed by PAHs (80.4 ng m⁻³), hopanes (9.38 ng m⁻³), and steranes (2.61 ng m⁻³). The low carbon preference index (CPI) of n-alkanes (mean: 1.30) indicates a predominantly anthropogenic origin. The PAH profile was dominated by high molecular weight (HMW) PAHs (4-ring and 5-ring compounds), constituting over 75% of the total, while low molecular weight (LMW) PAHs (2-ring and 3-ring compounds) made up only 5%, emphasizing the significant health risks posed by Dhaka's aerosols. Diagnostic ratios suggest that HMW PAHs were primarily associated with fossil fuel combustion, and hopanes were linked to traffic emissions. These findings underscore the urgent need for local and regional pollution control measures to reduce excessive anthropogenic aerosol emissions in South Asia.

Keywords: PM_{2.5}, organic compounds, anthropogenic emission, combustion,

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THE PRODUCTION OF HYDROGEN PEROXIDE BY ELECTROCHEMICAL OXYGEN REDUCTION REACTION AND APPLICATION OF FENTON REACTION IN ENVIRONMENTAL CATALYSIS

Chengbo Ma^a, Yang Li^a, Xiaobin Fan^a, Wenchao Peng^{a,*}

^a School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

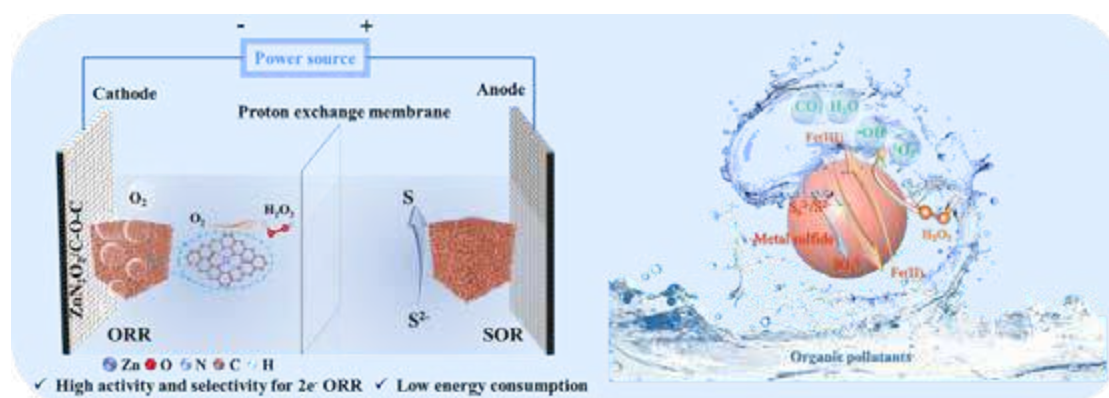
*Corresponding author: wenchao.peng@tju.edu.cn

Abstract

Fenton-like reaction is one of the most effective methods to treat organic wastewater. The reactive oxygen species generated by activated H_2O_2 can effectively remove refractory organic pollutants. H_2O_2 is currently produced using the anthraquinone method, which involves problems with high energy consumption and environmental pollution. The unstable property of H_2O_2 also raises the transportation cost and storage risk. The production of H_2O_2 via the electrochemical two-electron oxygen reduction reaction is regarded as an alternative route to the anthraquinone method due to its advantages of environmental benignity, high efficiency, and energy saving. Single-atom catalysts (SACs) are promising materials due to their adjustable electronic structure and maximum atomic utilization. More importantly, the distribution of metal sites at the atomic level can achieve the end-on type adsorption of O_2 rather than the side-on type, which reduces the possibility of O-O bond breaking. Zn SACs take on advantages in realizing the 2e^- ORR process, the zinc element with full-filled d-orbital can effectively avoid the formation of high-valence oxidative ions. In addition, zinc is inert for H_2O_2 activation, which effectively avoids the decomposition of H_2O_2 and electrode destruction caused by the $\cdot\text{OH}$. Experimental and theoretical calculations have confirmed that the coordination of adjacent C-O-C can effectively optimize the adsorption energy of $\text{Zn-N}_2\text{O}_2$ for $^*\text{OOH}$ and tune the 2e^- ORR selectivity. Moreover, a coupled system of anodic SOR and cathodic 2e^- ORR is fabricated, which can save 45% energy consumption compared to the OER- 2e^- ORR system. The Fenton system utilizes prepared H_2O_2 to degrade organic pollutants, and with a 100% pollutant removal ratio, it has the potential for practical application.

Keywords: oxygen reduction reaction, hydrogen peroxide, single-atom catalysts, Fenton reaction, environmental catalysis

Graphic / Image



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AMINE FUNCTIONALIZED GRAPHENE OXIDE DECORATED WITH ZNO-WO₃ NANOCOMPOSITES FOR REMEDIATION OF ORGANIC DYE FROM WASTEWATER

Md. Elias ^a, Mohammad Awlad Hossain ^{a*}

^aDepartment of Chemistry, Jagannath University, Dhaka 1100, Bangladesh

*Corresponding author: awlad1975@yahoo.com

Abstract

Photocatalytic degradation is as an efficient technique to eradicate toxic chemical pollutants from contaminated water sources. However, the selectivity and photocatalytic activity are the challenging targets to explore the new photocatalysts. Therefore, our research goal is to develop a suitable photocatalyst to satisfy the recent photocatalytic degradation demand. In this work, amine functionalized graphene oxide (NH₂-GO) supported heterojunction ternary novel nanocomposites (NH₂-GO/ZnO-WO₃) were prepared via simple solvothermal method. Structural and morphological investigations of the prepared composites are systematically observed by Field Emission Scanning Electron Spectroscopy (FE-SEM), X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR), and Ultraviolet-Visible (UV-vis) Spectroscopy. FT-IR analysis confirmed the effective functionalization of amine on graphene oxide. The XRD results indicated that the prepared nanocomposites were free from any impurities and the binary composite (NH₂-GO/ZnO) showed hexagonal wurtzite structure, whereas the ternary composite (NH₂-GO/ZnO-WO₃) exhibited mix crystal structure of monoclinic and hexagonal phase of WO₃ and ZnO, respectively. The synthesized ternary photocatalyst (NH₂-GO/ZnO-WO₃) demonstrated superior photocatalytic efficiency towards various organic dyes such as cationic dye methylene blue (MB, 85.89%) and anionic dye methyl orange (MO, 60.98%) compared to binary photocatalyst (NH₂-GO/ZnO) that showed only 52.28% of MB and 25.8% of MO dye degradation under UV light irradiation. The enhanced photocatalytic performance was mainly due to the low recombination rate of photogenerated electron-hole pair, narrow band gap, and large surface area of ternary composite. The presence of lone pair electrons in amino group provides a negative-charged surface composite resulting good interaction with cationic dye is the key to upgrade the photocatalytic performance. The ternary nanocomposite NH₂-GO/ZnO-WO₃ has the capacity to be a competent and acceptable photocatalyst for the photodegradation of organic dyes used in industries.

Keywords: Nanocomposite, Heterojunction, Photodegradation, Amine Functionalization, Organic dye

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RESEARCH ON ELECTROCATALYTIC CO₂ REDUCTION REACTION USING FUNCTIONAL COAL-BASED CARBON MATERIALS

Lang Xu*

*School of Chemical Engineering and Technology, China University of Mining and Technology
1 Daxue Road, Xuzhou, Jiangsu, 221116, China*

**Corresponding author: lang.xu@cumt.edu.cn*

Abstract

The electrocatalytic CO₂ reduction reaction (eCO₂RR) has been widely studied as it can convert CO₂ into high value-added chemicals using electricity generated from renewable energy sources. However, CO₂ molecules are structurally stable and difficult to be activated, which leads to small current densities and low product selectivities of electrocatalysts in the eCO₂RR processes. Coal has the advantages of natural robust carbon skeleton, excellent conductivity, and stability, making it suitable for preparing eCO₂RR electrocatalysts. Herein, we endow coal with abundant pore structure and active sites through activation and doping methods, transforming it into functional coal-based carbon material to enhance its eCO₂RR performance [1,2]. The spatial confinement effect of surface microporous structure of the functional coal-based carbon material can firmly anchor active species and enrich a large number of CO₂ molecules, while the robust carbon skeleton inside the material can rapidly transfer charges to the active sites. Therefore, the functional coal-based carbon material can intensify the charge/substrate interaction of the active sites, thereby enhancing the rate of eCO₂RR. On the other hand, multi-species doping can modulate the electronic structure of the active sites of the functional coal-based carbon material and improve the intrinsic activity of the active sites. The resulting highly active sites can optimize the adsorption strengths of CO₂/intermediates and lower their thermodynamic conversion energy barriers [3,4]. As a result, the coal-based carbon materials can not only convert CO₂ into CO or ethylene with high selectivity, but also achieve industrial-grade current densities, demonstrating its huge potential for commercial application. In addition, this work also provides a new research approach for enhancing the eCO₂RR performance of electrocatalysts by optimizing their geometric/electronic structure [5].

Keywords: CO₂ reduction; coal; confinement effect; electronic structure; industrial-grade current density.

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C-Au@TiO₂ NANOCOMPOSITE FOR ENHANCED PHOTODEGRADATION OF COMMERCIAL HENNA DYE

B.Karthikeyan ^{a*}, K.S.Ramya ^a, P.R Nithiasri ^a, J.Aarthi ^a

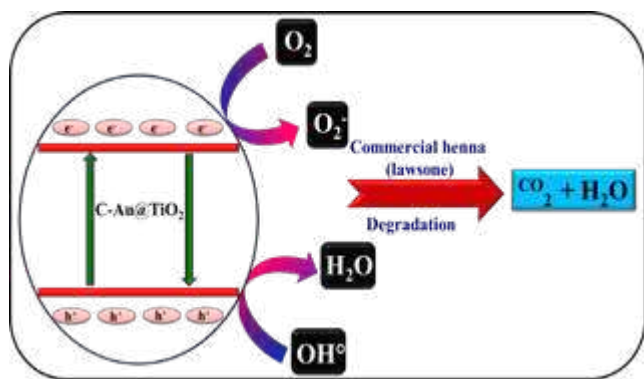
Department of Chemistry, Annamalai University, Annamalai Nagar, Chidambaram 608 002

*Corresponding author: bkarthi_au@yahoo.com

Abstract

In this study, TiO₂, Au@TiO₂, and C-Au@TiO₂ nanocomposites were successfully synthesized by using chemical co-precipitation method and characterized by XRD, FT-IR, FE-SEM, EDX, and UV-DRS techniques. XRD results confirmed the anatase phase of TiO₂ with successful incorporation of Au nanoparticles supported by carbon spheres. The FE-SEM images revealed spherical and aggregated nanosheet morphologies, while EDX analysis confirmed the elemental composition and homogeneity of the materials. UV-DRS analysis showed a significant redshift in absorption and a reduction in the bandgap energy upon Au and carbon doping, facilitating enhanced visible light absorption. The photocatalytic performance of the composites was evaluated using commercial henna (lawsone) dye under UV light irradiation. Among the materials tested, C-Au@TiO₂ exhibited superior photocatalytic activity, achieving 79% degradation efficiency after 90 minutes of UV irradiation. The enhanced performance is attributed to the synergistic effect of Au nanoparticles and carbon, which improved charge separation, increased surface area, and reduced electron-hole recombination. A plausible photocatalytic degradation mechanism is proposed, involving the generation of reactive oxygen species (ROS) like hydroxyl and superoxide radicals under UV light exposure, leading to the efficient breakdown of dye molecules. The incorporation of carbon further promoted charge mobility, enhancing the overall photocatalytic efficiency. The study suggests that the C-Au@TiO₂ nanocomposite is a promising material for environmental remediation applications, especially in the treatment of dye-contaminated wastewater. This work highlights the potential of noble metal and carbon modified semiconductor materials in addressing environmental pollution through sustainable and efficient photocatalytic strategies.

Keywords: Nanocomposite; C support; Band gap; environmental cleanup; water treatment



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CATALYTIC VALORIZATION OF CO₂ INTO CYCLIC CARBONATES: TOWARD SUSTAINABLE CARBON UTILIZATION

Suzaimi Johari^a, Mohd Rafie Johan^{a*}

^aNanotechnology and Catalysis Research Centre, Universiti Malaya

*Corresponding author: mrafiej@um.edu.my

Abstract

The increasing concentration of atmospheric CO₂ has driven global initiatives to develop sustainable technologies for its effective chemical conversion. One particularly promising approach is the catalytic conversion of CO₂ and epoxides into cyclic carbonates—high-value compounds used in polymers, pharmaceuticals, and energy storage. This reaction is notable for its 100% atom economy, mild operating conditions, and alignment with green chemistry principles. This analysis explores recent advances in the design and development of catalytic systems—both metal-based and metal-free—for the efficient synthesis of cyclic carbonates. Special emphasis is placed on bifunctional catalysts that combine Lewis acidic and nucleophilic sites to synergistically activate both CO₂ and epoxides. Key developments in homogeneous metal complexes (e.g., Al, Zn, Co) with tailored ligand frameworks, organocatalysts, and ionic liquids are discussed, alongside heterogeneous and supported systems that offer advantages in recyclability and process scalability. Mechanistic insights gained from kinetic studies and computational modeling will be highlighted to illustrate structure–activity relationships and to inform rational catalyst design. Additionally, green chemistry aspects—such as solvent choice, catalyst reusability, and energy efficiency—are considered, alongside emerging trends including continuous-flow processes and electrochemical CO₂ conversion. By integrating progress across diverse catalytic platforms, this contribution provides a critical perspective on the challenges and opportunities in CO₂ valorization through cyclic carbonate synthesis. The aim is to inform future catalyst development strategies and promote the transition toward sustainable chemical manufacturing.

Keywords: CO₂ utilization, cyclic carbonates, catalysis, green chemistry, epoxide cycloaddition

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INTEGRATING *SPIRULINA* PLATENSIS CULTIVATION AND AEROBIC COMPOSTING EXHAUST FOR CARBON MITIGATION AND BIOMASS PRODUCTION

Weidong Lu*

School of Chemistry and Civil Engineering, Shaoguan University

**Corresponding author: louiswdlu@163.com*

Abstract

Aerobic composting is an effective way to dispose of organic waste. However, considerable carbon is converted into CO₂ and emitted into the atmosphere, which is a waste of the carbon resource and has the potential for the greenhouse gas effect. In this study, an innovative approach coupling aerobic composting exhaust and *Spirulina platensis* cultivation has been proposed and investigated, resulting in a double-edged solution to mitigating waste and co-generating biomass with a minimal cost of CO₂ supplied in the culture. Experimental results showed that the maximum biomass productivity ranged from 56.61 to 58.38 mg·L⁻¹·day⁻¹ was achieved using aerobic composting exhaust as a carbon source. Moreover, the CO₂ fixation rates of 46.36 mg·L⁻¹·day⁻¹ and 76.81 mg·L⁻¹·day⁻¹ were obtained by *S. platensis* cultivation. Finally, the chemical composition analysis of *S. platensis* biomass obtained in an optimum condition showed an abundance of proteins and lipids, thereby indicating its great potential for biofuel industry.

Keywords: Composting exhaust; *Spirulina platensis*; Biomass production; Carbon mitigation; Biofuel

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QUALITY ASSESSMENTS OF REFINED, BLEACHED, AND DEODORIZED PALM OIL (RBDPO) AND REFINED USED COOKING OIL (RUCO) BASED ON FREE FATTY ACID (FFA) CONTENT FOR BIODIESEL PRODUCTION

Razan Mohd Razak, Faizuan Abdullah*, Farhana Ibrahim

Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia

**Corresponding author: faizuan@utm.my*

Abstract

The use of used cooking oil (UCO) as an alternative feedstock for the manufacturing of biodiesel has drawn more attention recently, especially as a substitute for palm oil, due to the increasing sustainability concerns and escalating global energy demands. The accurate measurement of the free fatty acid (FFA) content in the biodiesel feedstocks is essential to the production of biodiesel as it has a direct impact on the complexity and effectiveness of transesterification process. The objectives of this study were to develop and characterise an electrochemical sensor based on molecularly imprinted polymers (MIP) for the FFA detection, analyze and compare the FFA content in refined, bleached, and deodorized palm oil (RBDPO) and refined used cooking oil (RUCO) using the developed sensor, and assess the quality of biodiesel produced from both feedstocks. Based on a screen-printed carbon electrode (SPCE) modified with functionalized multi-walled carbon nanotubes (FMWCNT), zinc oxide nanoparticles (ZnONPs), and MIP, the fabricated electrochemical sensor offers a viable substitute for traditional titration techniques, which are frequently labour-intensive, time-consuming, environmentally unsustainable, and prone to human error. Oleic acid served as the template molecule and methacrylic acid (MAA) as the functional monomer. The sensor was successfully fabricated and modified, as confirmed by its characterization using attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR), atomic force microscopy (AFM), field emission scanning electron microscopy with energy dispersive X-ray spectroscopy (FESEM-EDX), thermogravimetric-differential thermal analysis (TGA-DTA), and cyclic voltammetry (CV). The MIP sensor surpassed the titration method in terms of sensitivity based on the performance evaluation. The MIP sensor possessed the limit of detection (LOD) and limit of quantification (LOQ) of 0.1718 mM and 0.5206 mM, respectively, with a coefficient of determination (R^2) of 0.9951. Meanwhile, the titration method produced LOD of 0.9420 mM and LOQ of 2.8545 mM with an R^2 of 0.9000. When used an actual sample, the MIP sensor demonstrated limited reliability despite the improved analytical parameters. This was due to the intricate matrix effects in RBDPO and RUCO, which hindered the accurate measurement of FFA levels. The biodiesel synthesized from RBDPO complied with all quality requirements outlined in the EN 14214 specifications, except for a slightly elevated group I metals concentrations that remained within acceptable regulatory limits. However, biodiesel produced from RUCO failed to meet the EN 14214 specifications due to an incomplete transesterification reaction, signifying that the feedstock must be further pre-treated. Overall, the findings highlight the potential of MIP-based sensors for quick FFA analysis, while also emphasize the need for further optimization and sample pre-treatment to ensure accuracy in complex matrices.

Keywords: Electrochemical sensor; molecularly imprinted polymer sensor (MIPS); screen-printed carbon electrode (SPCE); free fatty acid (FFA); biodiesel; transesterification.

INSIGHT INTO THE EFFECT OF EDTA ON PHOTOCATALYTIC PERFORMANCE OF BISMUTH-BASED MATERIALS

Qiaofeng Han*, Huiwei Ding

Key Laboratory for Soft Chemistry and Functional Materials, Ministry of Education, Nanjing University of Science and Technology, Nanjing 210094, China

**Corresponding author: hanqiaofeng@njust.edu.cn*

Abstract

For the photocatalytic system of bismuth-based materials, ethylenediaminetetraacetic acid disodium salt (EDTA-2Na) is often used as a hole (h^+) trapping agent for the investigation of photocatalytic mechanism due to its significant chelating effect and strong electron-donating ability. For instance, if the addition of EDTA-2Na induced a decrease in the photocatalytic activity, the h^+ are regarded as the main active species.^{1,2} Herein, our work suggests that the effect of EDTA-2Na on the photocatalytic performance of bismuth-based compounds varies with the chemical compositions. For those with high Bi/anions ratios such as Bi_2O_3 and $\text{Bi}_5\text{O}_7\text{I}$, the addition of a certain amount of EDTA-2Na could significantly improve photocatalytic activity, and whereas, the change in the photocatalytic activity BiOX ($\text{X} = \text{Br}, \text{I}$) and $\text{Bi}_2\text{O}_2\text{CO}_3$ with low Bi/anion ratios wasn't significant. Conversely, BiVO_4 and Bi_2MoO_6 with lower Bi/anion ratios exhibited even worse photocatalytic performance after adding EDTA-2Na. The investigation on the photocatalytic mechanism suggests that the ability of EDTA-2Na to transfer electrons from its HOMO energy levels to the conduction band (CB) of bismuth-based compounds competes with that to fill the electron into the valence band (VB). Because the CB mainly consists of Bi 5p orbitals and the VB is mostly contributed by the hybrid orbitals of Bi 6s and O 2p or other non-metal elements,³ for those with high Bi/anions ratios, stronger coupling effect between CB and HOMO energy levels of EDTA-2Na could generate, which benefits the migration of electrons from EDTA to CB and then reacts with O_2 to generate $\cdot\text{O}_2^-$ while maintaining the h^+ . Therefore, their photocatalytic activity would be improved. Otherwise, the electrons on HOMO energy levels of EDTA would transit to VB and trap the holes, which is adverse to the hole-dominant photocatalysis process.

Keywords: bismuth-based photocatalyst, EDTA-2Na, Bi/anions ratios, coupling, electron migration

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NOVEL PHOSPHOTUNGSTIC ACID MODIFIED ACTIVATED CARBON DERIVED FROM PALM BIOMASS FOR REMOVAL OF ORGANIC DYES FROM WASTEWATER

Abdullah M. Aldawsari*

Department of Chemistry, College of Science and Humanities, Prince Sattam Bin Abdulaziz University, Al-kharj, Saudi Arabia

**Corresponding author: abdullah.aldawsari@psau.edu.sa*

Abstract

Water pollution by dyes is a significant environmental issue, primarily due to the extensive use of synthetic dyes in industries such as textiles, leather, paper, plastics, and cosmetics [1]. However, its presence in wastewater poses significant risks to aquatic ecosystems and human health. Methylene blue toxicity, potential carcinogenicity, and non-biodegradable nature make it a significant pollutant in water environments [2]. magnetite nanoparticle decorated graphene oxide (MGO,3]. As a result, Effective removal from wastewater is crucial to mitigate these risks and protect aquatic ecosystems and human health. In this study, a novel phosphotungstic acid-modified activated carbon (TPA@DPAC) was successfully synthesized to enhance the removal efficiency of methylene blue from water. The structures of DPAC and TPA@DPAC were characterized using FTIR, SEM, EDX, TEM, XRD, and BET surface area analyses. Adsorption tests were performed under various conditions, including contact time, solution pH, initial MB concentration, temperature, and adsorbent dosage. Results indicated that TPA@DPAC achieved a higher removal efficiency (99.07%) compared to DPAC (90.54%) under optimal conditions (dose: 0.02 g, pH: 6.0, MB concentration: 25 mg/L, temperature: 298 K, agitation speed: 100 rpm). The Freundlich model ($R^2 = 0.997$) provided the best fit for both adsorbents, indicating multilayer adsorption behavior, with a maximum adsorption capacity of 321.04 mg/g for TPA@DPAC and 263.52 mg/g for DPAC at 25 °C. The adsorption kinetics followed a PFO model ($R^2 = 0.995$) for MB adsorption onto DPAC, while MB adsorption onto PTA@DPAC aligned with the Elovich model. In conclusion, phosphotungstic acid-modified activated carbon was an effective adsorbent for removing MB from water.

Keywords: Methylene blue; phosphotungstic acid; activated carbon; adsorption

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SEWAGE SLUDGE AS ALTERNATIVE SUBSTRATE FOR BIOCHAR PRODUCTION AIMED AT CO₂ CAPTURE

Sandro Froehner^{a,*}, Miguel Aisse^b, Marcos Capitolino Barros Filho^b, Marcelo Errera^a,

^a*Department of Environmental Engineering, Federal University of Parana, Brazil.*

^b*Department of Hydraulics and Sanitation, Federal University of Parana, Brazil.*

**Corresponding author: froehner@ufpr.br*

Abstract

Sludge, the solid byproduct of sewage treatment, presents a significant challenge for sanitation companies due to the complexities of its treatment and high operational and disposal costs. Global sludge production is projected to reach 150 to 200 million tons by 2025, according to the literature. Effective management of sewage sludge and the development of innovative technologies to mitigate atmospheric greenhouse gas emissions are essential for environmental protection and safeguarding human and animal health. In this study, a thermal drying process was applied to sewage sludge, utilizing methane produced during wastewater treatment as an energy source. This approach created a favorable feedstock for biochar production. Biochar, known for its high efficacy in adsorbing GHGs like CO₂, was produced via slow pyrolysis at 600°C, with the final temperature held for 1 hour. The biochar was characterized using Fourier-transform infrared (FTIR) spectroscopy and Raman spectroscopy. FTIR analysis revealed that many chemical functional groups present in the sewage sludge were preserved in the biochar, indicating that pyrolysis did not completely degrade these groups. Raman spectra demonstrated a structural transformation from an amorphous phase to graphene-like arrangements, featuring an ordered configuration with some structural defects. The CO₂ adsorption capacity of the biochar was evaluated using a fixed-bed column experiment, yielding a value of 4.24 mol kg⁻¹. This performance is comparable to other sewage sludge-derived biochars but lower than that of lignocellulosic biochars. The asymmetry observed in the breakthrough curve suggests heterogeneity in the biochar bed, likely attributable to variations in particle size and pore structure. These findings highlight the significant potential of sewage sludge-derived biochar as a cost-effective and sustainable material for CO₂ adsorption. Further optimization of production parameters and investigation of its performance under various operational conditions could enhance its applicability in carbon capture and storage technologies.

Keywords: sludge, biochar, sustainability, greenhouse gases

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ULTRA-THIN $\text{FeCo}(\text{OH})_x$ PRECURSOR-DERIVED CO-DOPED Fe_3O_4 NANOPARTICLES ON N-DOPED GRAPHENE AS HIGHLY STABLE OXYGEN ELECTROCATALYST

Sunglun Kwon*

Department of Chemistry, The Catholic University of Korea, Bucheon, 14662, Korea

**Corresponding author: kwonsl@catholic.ac.kr*

Abstract

Developing efficient and cost-effective catalysts for the oxygen reduction reaction (ORR) is essential for advancing electrochemical energy technologies. This study introduces a novel synthesis route for spinel $\text{Fe}_x\text{Co}_{3-x}\text{O}_4$ nanoparticles (~30 nm) anchored on N-doped reduced graphene oxide (NRGO). A solvothermal process in formamide was used to produce ultrafine $\text{FeCo}(\text{OH})_x$ (~5 nm) nanoparticles, which were uniformly dispersed on NRGO. These nanoparticles served as precursors for spinel $\text{Fe}_x\text{Co}_{3-x}\text{O}_4$ formation through high-temperature annealing at 900°C. The incorporation of Co^{2+} ions into the synthesis process played a critical role in inhibiting the rapid oxidation of Fe^{2+} to Fe^{3+} , thereby promoting the formation of Fe_3O_4 over Fe_2O_3 . This strategy enabled the creation of well-dispersed, highly stable $\text{Fe}_x\text{Co}_{3-x}\text{O}_4$ nanoparticles with minimal aggregation, even after annealing.

The resulting $(\text{Co})\text{Fe}_3\text{O}_4$ -NRGO nanocomposite exhibited remarkable ORR performance, achieving a current density of $5.01 \text{ mA} \cdot \text{cm}^{-2}$ at 0.75 V vs. RHE and an electron transfer number of ~3.7, values comparable to those of commercial Pt/C catalysts. Furthermore, the catalyst demonstrated exceptional durability, retaining 58% of its initial current density after 40,000 s of continuous operation, significantly outperforming Pt/C, which retained only 25%. This superior performance is attributed to the robust interaction between the $(\text{Co})\text{Fe}_3\text{O}_4$ nanoparticles and the NRGO support, facilitated by the Co ion precursor during synthesis and annealing.

These findings highlight the potential of this synthesis approach to produce highly efficient, stable, and cost-effective ORR catalysts, offering a promising alternative to conventional Pt-based materials for energy applications such as fuel cells.

Keywords: Layered double hydroxide nanosheet, Oxygen reduction reaction, Electrocatalysis

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IN SILICO* BINDING AFFINITY ANALYSIS OF PCBs WITH TCE REDUCTIVE DEHALOGENASE FROM *Sulfurospirillum multivorans

Alexandrea Beatriz G. Manangan^{a,b*}, Nelson R. Villarante^b, Junie B. Billones^b

^aNational Institutes of Health, University of the Philippines Manila

^bCollege of Arts and Sciences, University of the Philippines Manila

*Corresponding author: agmanangan@up.edu.ph

Abstract

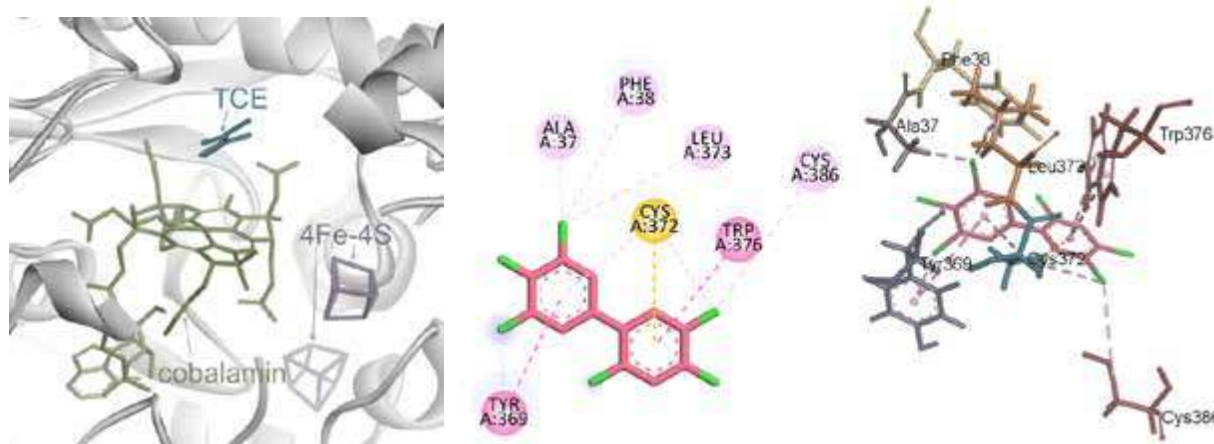
Polychlorinated biphenyls (PCBs) are persistent organic pollutants (POPs) which have been used worldwide due to their chemical stability and dielectric properties. Although its production has been banned since the 1970s, many PCBs are still in existence in the environment, including soils and marine sediments. Current remediation technology for PCB-contaminated environments is highly destructive and unsustainable, hence, there is a need to conduct alternative strategies for PCB degradation. In this study, the degradation of 20 PCBs with TCE RDase from *S. multivorans* was explored through molecular docking. This will be beneficial in elucidating vital information for the degradation and modification of PCBs.

Successful binding of the PCB congeners in the binding pocket of the enzyme revealed that PCB-167 and 180 had the highest binding energy values for PceA without the cobalamin cofactor, whereas PCB-123, PCB-77 and PCB-126 had the largest binding energy for PceA with the cofactor. Observation of the enzyme-ligand factors revealed mostly hydrophobic enzyme-ligand interactions and preferential interactions with meta and para chlorines. Pearson correlation analysis revealed MW and log BCF values as moderately correlated and KOA as strongly correlated parameters for PceA without cobalamin; meanwhile, the enzyme with the cofactor showed poor but positive correlations.

To gain more insight on PceA enzyme from *S. multivorans*, it is recommended that all 209 PCBs are assessed through molecular docking. Different PDB structure data of the enzymes may also be utilized to validate binding mechanisms and enzyme-ligand interactions. QSAR analysis can be employed to reveal the correlation of the structural data with other descriptors of PCBs.

Keywords: polychlorinated biphenyls, reductive dehalogenases, molecular docking, *Sulfurospirillum multivorans*, bioremediation

Graphic / Image



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ASSESSMENT OF ORGANOCHLORINE PESTICIDE RESIDUES IN AGRICULTURAL SOILS OF SOUTHERN NIGERIA AND ANALYSIS OF POTENTIAL HEALTH RISKS

Imeobong U. Udoekpo^{1,2}, Akwaowo I. Inyangudoh^{1,2,3*}, Treasure A. Awa-Arua^{1,2}, Ekeoma I. Ogwo⁴, Nnanake-Abasi O. Offiong⁵, Edu J. Inam^{1,2*}, Crispin J. Halsall⁴

¹ Department of Chemistry, University of Uyo, Uyo, Nigeria

² Centre for Energy and Environmental Sustainability Research, University of Uyo, Uyo, Nigeria

³ Department of Chemistry, Faculty of Physical Sciences, Akwa Ibom State University, Ikot Akpaden, Akwa Ibom State, Nigeria

⁴ Lancaster Environment Centre, Lancaster University, Lancaster, LA1 4YQ, UK

⁵ Department of Chemical Sciences, Faculty of Computing & Applied Sciences, Topfaith University, Mkpatak – 530109, Nigeria

*Corresponding Authors: akwaowoinyangudoh20@gmail.com; eduinam@uniuyo.edu.ng

Abstract

The use of pesticides in commercial farms can lead to exposure among various vulnerable groups. This study assessed the distribution, human health risks, and origins of 13 targeted organochlorine pesticides (OCPs) in soil samples from commercial farms in Southern Nigeria. Following a questionnaire survey on pesticide usage, soil samples were subjected to Soxhlet extraction and analyzed using gas chromatography-mass spectrometry. Results indicated that 31.6% of farmers did not use personal protective equipment, and only 37.6% had received training on safe pesticide applications. While pyrethroids and organophosphates were commonly used, organochlorines were rarely applied. The detected levels of OCPs in the agricultural zones ranged from below detection limit (BDL) to $18.35 \pm 13.83 \mu\text{g/kg}$ and were generally within the minimum risk level (MRL), except for α -HCH and β -HCH in Oron and Etinan zones. The estimated non-carcinogenic risks from detected OCPs were insignificant at the time of the study, as the calculated Hazard Indexes (HIs) and Hazard Quotients (HQs) for ingestion, dermal absorption, and inhalation were all less than 1, indicating generally low risks. The carcinogenic risk assessment showed that the Incremental Lifetime Cancer Risk (ILCR) values ranged from 10^{-10} to 10^{-4} , indicating a very low to low risk level according to the classification by the United States Agency for Toxic Substances and Disease Registry (US ATSDR). Source apportionment suggested that most OCP congeners were of historical origin, with only a few indicating recent use. In conclusion, organochlorine pesticide residues in the studied farms posed minimal health risks, with most originating from historical rather than recent use.

Keywords: Agricultural soils; organochlorine pesticide; public health; risk assessment; southern Nigeria

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SUBSTITUENT EFFECTS IN BENZOYL THIOUREA-BASED CHEMOSENSORS FOR SELECTIVE COPPER (II) ION DETECTION

Hua Yong Goh^a, Ming Yueh Tan^a, Siew San Tan^{a*}

^aDepartment of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Kelang, Setapak, 53300 Kuala Lumpur, Malaysia.

*Corresponding author: siewsan@taru.edu.my

Abstract

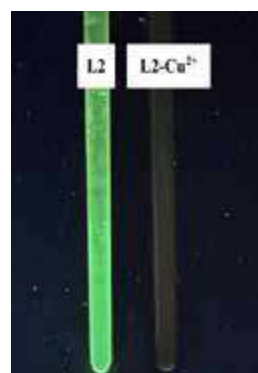
Three *para*-substituted benzoyl thiourea-based chemosensors, **L1** (H), **L2** (Me), and **L3** (Br), incorporating 2-aminobenzothiazole, were synthesized and characterized using FT-IR, UV-Visible, CHNS, DSC, and NMR spectroscopy (¹H and ¹³C). Their fluorescence and colorimetric sensing abilities were evaluated against various metal ions, with all ligands exhibiting high selectivity toward Cu²⁺ ions, displaying turn-off fluorescence and a color change from colorless to yellow due to chelation-enhanced quenching (CHEQ).¹ Among the three ligands, **L2** demonstrated the best sensing performance, with the lowest limit of detection (LOD) at 0.96 μM (UV-Visible) and 6.00 μM (fluorescence), compared to **L1** (0.99 μM, 10.10 μM) and **L3** (1.25 μM, 11.53 μM). The chemosensors exhibited 1:1 binding stoichiometry with Cu²⁺ ions, coordinated through two NH moieties in the ligand framework. Among them, **L2** had the highest binding constant (*K_b*) of 11.52 × 10⁴ M⁻¹, followed by **L1** (8.67 × 10⁴ M⁻¹) and **L3** (8.41 × 10⁴ M⁻¹), confirming its stronger Cu²⁺ binding affinity. The superior performance of **L2** was attributed to the electron-donating effect of the methyl group, which increased electron density and enhanced binding affinity and sensitivity toward Cu²⁺ ions.² DFT calculations further supported these findings, revealing that Cu²⁺ complexation significantly reduced the HOMO-LUMO energy gap, facilitating electron delocalization.³ **L2**-Cu²⁺ had the lowest energy gap (1.68 eV), compared to **L1**-Cu²⁺ (1.93 eV) and **L3**-Cu²⁺ (2.17 eV), further explaining its superior sensing performance. To enable practical application, test strips were prepared by impregnating filter paper with a DMSO solution of the chemosensor. These strips successfully detected Cu²⁺ ions in water, producing a noticeable color change from colorless to yellow. These findings highlight the critical role of substituent effects in Cu²⁺ ions sensing, with **L2** emerging as the most effective chemosensor for environmental monitoring applications.

Keywords: benzoyl thiourea-based, substituent effects, turn-off fluorescence, test strips

Structure of L2.



Luminescence of L2 and L2-Cu²⁺.



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ROLE OF THERMAL ADAPTATION BEHAVIORS ON THE CHARACTERISTICS AND RESPIRATORY DISPOSITION OF INDOOR AIRBORNE MICROPLASTIC

Chien-Cheng Jung^{a*}, Pei-Wei Yeh^a

^aDepartment of Public Health, China Medical University, Taichung, China

*Corresponding author: ccjung@mail.cmu.edu.tw

Abstract

Global warming has increased the frequency of thermal adaption behaviors indoors, which in turn alters indoor airflow patterns. However, whether such behaviors affect the variation and respiratory deposition of airborne microplastics (MPs) indoors has yet to be fully investigated. Indoor and outdoor MP samples were collected from homes with air conditioner (UAC) or without air conditioner (NAC) and with electric fan (UFAN) or without electric fan (NFAN) conditions to assess their impacts. Our data showed that the major shapes, sizes, and polymer compositions of MPs were fragment, 3 to 50 μm , and polyamide in indoor and outdoor air, respectively, regardless of thermal adaptation behaviors. The ratios of indoor and outdoor MP concentrations were significantly higher under the UFAN (1.26) condition compared to UAC (0.61), NAC (0.68), and NFAN (0.73) conditions (Figure 1). A generalized estimation equation indicated that the ratio in the UFAN condition was 1.15 times that of the reference (NAC and NFAN). A multiple-path particle dosimetry modeling showed that the deposition of smaller-sized MPs was significance in the deep lung in the UFAN condition (Figure 2). Outdoor MP concentrations were positively correlated with both outdoor temperature and indoor MP concentrations. This study indicated that thermal degradation may lead to the release of MPs outdoors, which then contributes to indoor air. Electric fan usage further increased indoor MP concentrations and exposure in the deep lung. These findings reveal that thermal adaptation behaviors change indoor MP exposure, with implications for climate adaptation strategies and indoor air quality management.

Keywords: indoor air, microplastic, thermal adaptation behavior, thermal degradation

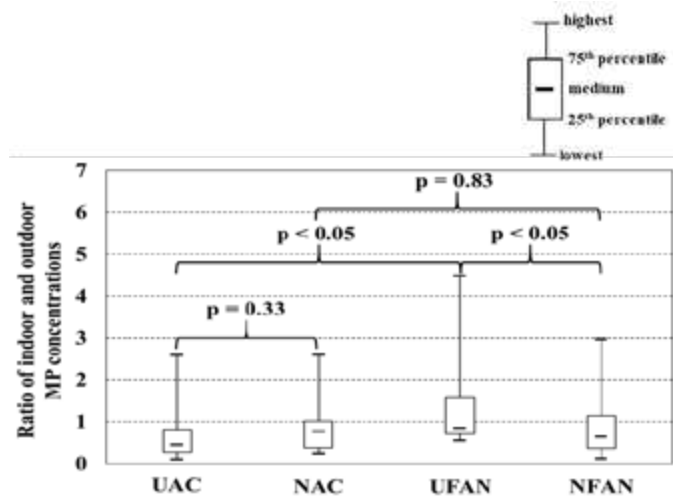


Figure 1. Box plots of ratios of indoor and outdoor MP concentrations according to different thermal adaptation behaviors.

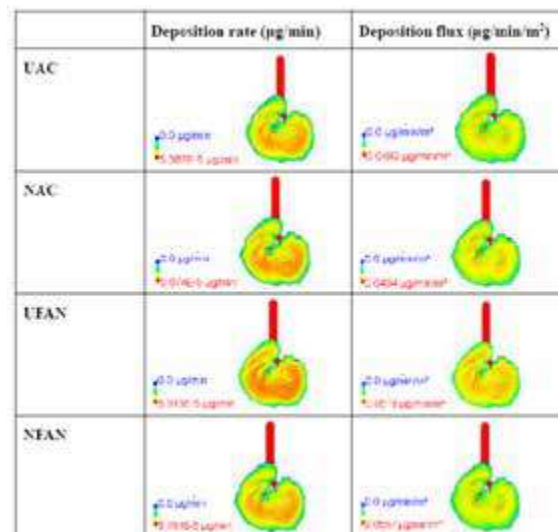


Figure 2. Deposition rate and flux of indoor MPs exposure in MPPD model according to different thermal adaptation behaviors.

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DISPERSANT-ASSISTED VOLUME REDUCTION OF RADIOCESIUM-CONTAMINATED SOIL

**Zinnat A. Begum^{a,*}, Rashedul Islam Ripon^b, Iqbal Hossain^b, Abhijit Barua^b,
 Ismail M.M. Rahman^a**

^a *Institute of Environmental Radioactivity, Fukushima University, 1 Kanayagawa, Fukushima City, Fukushima 960-1296, Japan*

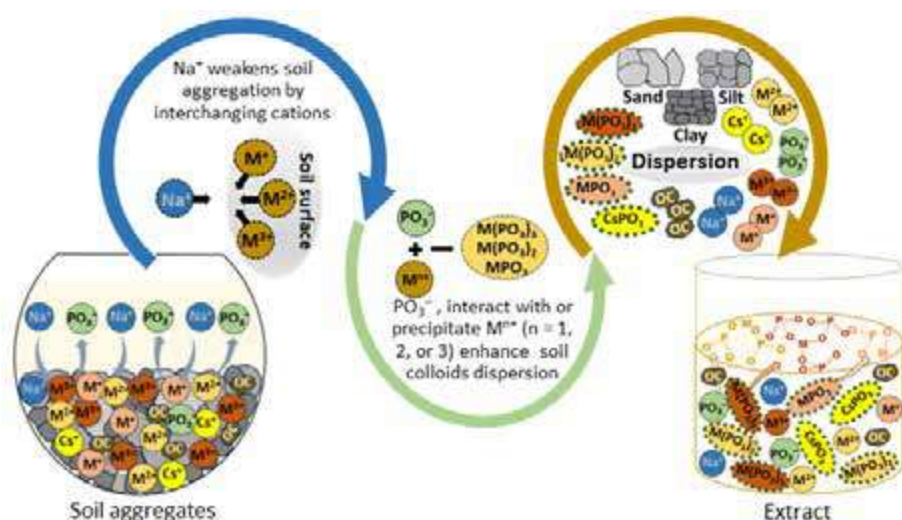
^b *Graduate School of Symbiotic Systems Science and Technology, Fukushima University, 1 Kanayagawa, Fukushima City, Fukushima 960-1296, Japan*

*Corresponding author: zinnat.ara@gmail.com

Abstract

The Fukushima Daiichi Nuclear Power Plant (FDNPP) accident in 2011 resulted in the release of radionuclides, including radiocesium (r-Cs: ^{137}Cs), leading to widespread soil contamination. Effective volume reduction of contaminated soil is crucial for efficient remediation and disposal. This study investigates the use of a dispersing agent to enhance the separation of r-Cs contaminated fine soil particles from larger particles, thereby facilitating volume reduction. This research aims to: (1) evaluate the effectiveness of sodium hexametaphosphate (SHMP) as a dispersing agent for volume reduction of r-Cs-contaminated soil; (2) investigate the interaction and retention behavior of r-Cs with soil components before and after dispersion with water and SHMP. Soil samples from Fukushima Prefecture were treated with water and SHMP. Wet sieving was performed to separate soil size fractions. The activity concentration of ^{137}Cs in different size fractions was measured using a high-purity germanium detector. Soil properties and the distribution of ^{137}Cs , ^{133}Cs , and organic carbon (OC) in soil solid phases were analyzed. Fourier transform infrared spectroscopy was used to characterize soil functional groups. SHMP effectively dispersed clay and silt particles, concentrating r-Cs into the finer soil fractions ($< 212\ \mu\text{m}$). A strong negative correlation was observed between OC and ^{137}Cs in the clay and silt fraction of SHMP-treated soil. The dissolution of polyvalent metal ions (Ca^{2+} , Mg^{2+} , Al^{3+} , Fe^{3+}) was positively correlated with the release of OC in the presence of SHMP. SHMP-assisted wet sieving effectively concentrates r-Cs into a smaller soil volume fraction, suggesting its potential for volume reduction of contaminated soil. The findings contribute to developing efficient remediation strategies for r-Cs contaminated areas.

Keywords: radiocesium; sodium hexametaphosphate; volume reduction



Presumed mechanism: SHMP-assisted volume reduction of ^{137}Cs -contaminated soil

SELECTIVE SEPARATION OF RADIOSTRONTIUM FROM CONTAMINATED WATER USING A CROWN ETHER-FUNCTIONALIZED MESOPOROUS SILICA SORBENT

Ismail M. M. Rahman^{a,*}, Rashedul Islam Ripon^b, Iqbal Hossain^b, Abhijit Barua^b,
Zinnat A. Begum^a

^a Institute of Environmental Radioactivity, Fukushima University, 1 Kanayagawa, Fukushima City, Fukushima 960-1296, Japan

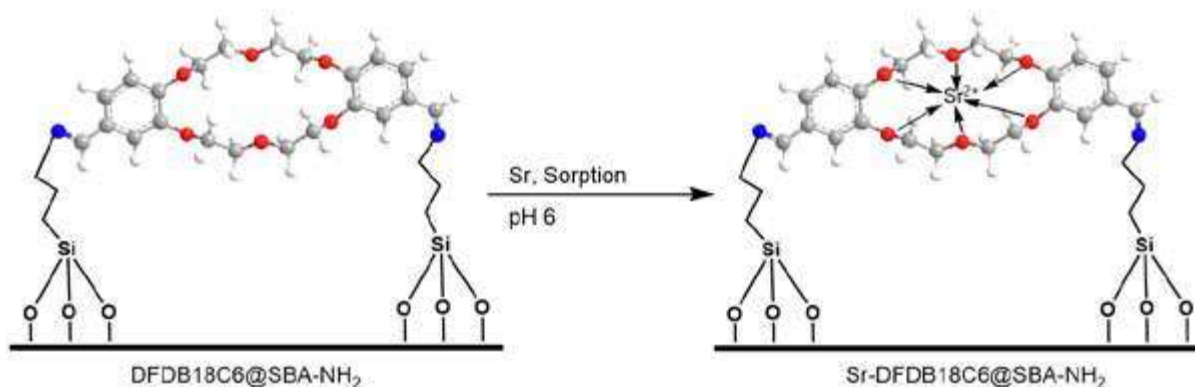
^b Graduate School of Symbiotic Systems Science and Technology, Fukushima University, 1 Kanayagawa, Fukushima City, Fukushima 960-1296, Japan

*Corresponding author: immrahman@ipc.fukushima-u.ac.jp

Abstract

The release of radiostrontium (r-Sr: ^{90}Sr) during nuclear accidents poses significant environmental and health risks due to its long half-life and chemical similarity to calcium, which allows it to enter the food chain and cause serious health issues in humans. This study aimed to develop a novel sorbent, DFDB18C6@SBA-NH₂, for the efficient and selective removal of r-Sr from wastewater. The sorbent was synthesized by immobilizing diformal dibenzo-18-crown-6-ether (DFDB18C6) onto amino-modified mesoporous silica (SBA-NH₂). Batch sorption experiments were conducted to evaluate the effects of pH, contact time, initial Sr concentration, and temperature on r-Sr sorption. The sorbent's potential for real-world applications was also tested with actual contaminated water from the Chernobyl Nuclear Power Plant (ChNPP) cooling pond (CP). The DFDB18C6@SBA-NH₂ sorbent demonstrated excellent selectivity for r-Sr, with a maximum sorption capacity of 2.75 mg g⁻¹. The sorption process followed pseudo-second order kinetics and the Langmuir isotherm model, indicating chemisorption and monolayer coverage. Thermodynamic studies revealed the endothermic nature of the sorption process. The sorbent achieved a remarkable 99.7% removal rate for ^{90}Sr from ChNPP CP water over five sorption cycles, even in the presence of competing ions. The newly developed DFDB18C6@SBA-NH₂ sorbent exhibits high efficiency and selectivity for removing r-Sr from wastewater, including real-world samples from the ChNPP CP. The sorbent's strong performance and its environmentally friendly nature make it a promising candidate for the remediation of r-Sr from contaminated water sources. Further research can explore its potential applications in other contaminated sites and its long-term stability.

Keywords: radiostrontium, separation, sorption, wastewater, solid-phase sorbent



Proposed mechanism of Sr sorption onto DFDB18C6@SBA-NH₂

SOLVENT EXTRACTION SEPARATION OF COBALT-IRON BINARY SYSTEMS IN NITRIC ACID MEDIA USING TRIALKYLAMINE EXTRACTANTS

Bo Zhang^{a,*}, Ding Ding^a

^a*Institute of Physical and Chemical Engineering of Nuclear Industry*

*Corresponding Author: ‡zhangbo2017@tju.edu.cn

Abstract

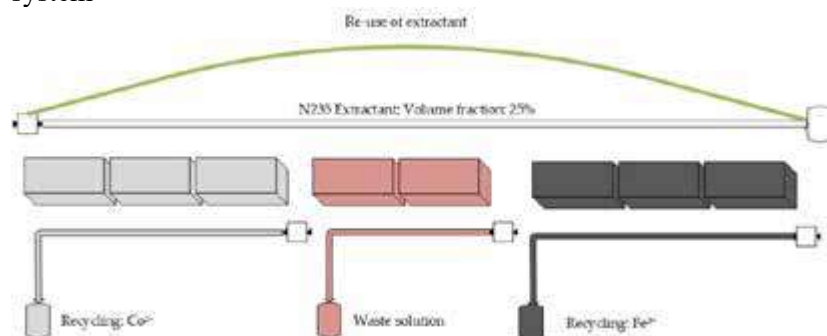
To address the critical need for sustainable recovery of strategic metals from decommissioned Fe-Co alloys, this study systematically investigates cobalt-iron separation dynamics in nitric acid media using trioctylamine (N235)-based solvent extraction. A comprehensive parametric optimization was conducted through controlled chloride ion regulation via NH_4Cl addition, examining the interplay between initial acidity (0.5-3.0 mol/L HNO_3), chloride concentration (0.1-1.2 mol/L), and extractant composition (5-30 vol% N235 in sulfonated kerosene).

Key findings reveal:

1. Extractant selectivity: N235 exhibited preferential iron (III) extraction with distribution coefficients (D_{Fe}) increasing exponentially from 2.1 to 18.7 as $[\text{Cl}^-]$ elevated from 0.5 mol/L to 1.2 mol/L, while cobalt (II) remained predominantly in aqueous phase ($D_{\text{Co}} < 0.05$).
2. Phase behavior: A 25 vol% N235 formulation achieved optimal separation efficiency ($\beta\{\text{Fe/Co}\} = 387 \pm 12$) at 1.0 mol/L Cl^- , with $< 2\%$ co-extraction of cobalt.
3. Stripping kinetics: Quantitative iron recovery ($> 99\%$) occurred at 0.05 mol/L H_2SO_4 , while higher acidities (> 0.1 mol/L) induced phase emulsification due to interfacial tension collapse.

Multi-stage counter-current extraction simulations confirmed that a 3-stage configuration (A/O = 1:1.5) produced cobalt solutions with 99.97% purity and cobalt recovery exceeding 99.5%. This methodology provides a technically viable pathway for nuclear/energy sector metal recycling with minimized secondary waste generation.

Keywords: Hydrometallurgy; Liquid-liquid extraction; Critical metal recovery; Trioctylamine; Nitric acid-chloride system



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EFFICIENT ORGANIC SOLVENT NANOFILTRATION MEMBRANE FOR MOLECULAR SIEVING

Hilal Ahmad^{a,*}, Abdul Waheed^a, Isam H. Aljundi^{a,b}

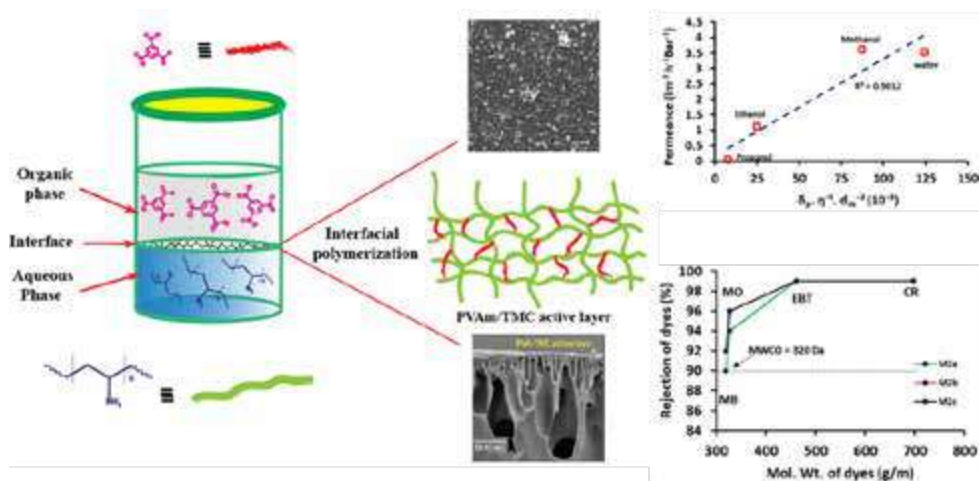
^a *Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, 31261, Saudi Arabia*

^b *Chemical Engineering Department, King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, 31261, Saudi Arabia*

*Corresponding author: hilal.ahmad@kfupm.edu.sa

Abstract

Recovering and reusing organic solvents are critical challenges in laboratory and industrial chemical processes [1-3]. To address these challenges, membrane-based separations have emerged as a highly effective solution, particularly for purifying contaminated solvents or isolating target compounds [4,5]. In this study, we employed polyvinyl amine (PVAm) as an aqueous monomer, crosslinked with trimesoyl chloride (TMC) as an organic phase monomer, to fabricate a polyamide active layer on polyacrylonitrile support. A set of 9 membranes was prepared for optimizing the membrane structure by varying the PVAm concentration and duration of interfacial polymerization (IP). It was found that increasing the PVAm concentration or IP duration resulted in increasing the rejection and lowering the permeance of the membranes. This was due to decreasing molecular weight cut-offs (MWCOs) of the membranes. Among different membranes, M2a was found to be best optimized with an MWCO of 350 Da and demonstrated superior rejection capabilities, exceeding 99% for congo red and Erichrome black T, while 93% and 90% for methyl orange and methylene blue, respectively. Among the polar solvents, methanol achieved the highest permeance of 3.8 L m⁻² h⁻¹ bar⁻¹, while n-hexane, a non-polar solvent, showed a permeance of 4.2 L m⁻² h⁻¹ bar⁻¹. This study highlights the potential of polymeric amines, varying their concentrations and duration of IP in developing efficient organic solvent nanofiltration membranes.



Keywords: Interfacial polymerization; Polyvinyl amine; Polar and non-polar solvents; Permeance and rejection

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VALORIZATION OF BIOCHAR AND COW DUNG FOR HYDROCARBON REMEDIATION: IMPLICATIONS FOR CARBON SEQUESTRATION AND SUSTAINABLE SOIL RESTORATION

Paschal Okiroro Iniaghe^{a*}, Faustina Onyeyirichi Iniaghe^b, Godswill Okeoghene Tesi^b,
Wisdom Iwurie^b

^aFederal University Otuoke, Nigeria

^bFederal University of Petroleum Resources Effurun, Nigeria

*Corresponding author: iniaghepo@fuotuo.ke.edu.ng

Abstract

Biochar and cow dung have recently gained attention as cost-effective and sustainable materials for environmental remediation. Their unique properties enable effective hydrocarbon removal from contaminated soils while contributing to carbon sequestration and restoration of soil health. This study characterized rice husk biochar (RHB), cow horn biochar (CHB), and cow dung (CD) to evaluate their hydrocarbon adsorption potential and explore their roles in carbon retention in soil. X-ray diffraction (XRD) was used to determine mineral composition, while X-ray fluorescence (XRF) analyzed oxide composition. Brunauer-Emmett-Teller (BET) measurements were conducted to assess surface area and porosity, and Fourier-transform infrared spectroscopy (FTIR) was employed to identify functional groups responsible for adsorption. XRD showed that RHB contained 65% graphite, while CHB contained 56% graphite, indicating their potential as stable carbon reservoirs. For CD, it contained 56% carbon (as chaoite), along with urea (18%) and ammonium phosphate (24%), suggesting additional nutrient benefits for soil restoration. Oxide composition analysis revealed distinct differences in CaO (4.45%, 17.26% and 27%), SO₃ (0.57%, 30.17% and 2.87%), and K₂O (7.24%, 2.46% and 37.6%) for RHB, CHB and CD, respectively. BET analysis showed that CHB had the highest surface area (356 m² g⁻¹), followed by RHB (254.9 m² g⁻¹) and CD (185.9 m² g⁻¹), with mesoporous structures (pore diameters ~2.55-2.65 nm). FTIR confirmed Si-O-Si stretching in RHB and hydroxyl (-OH) functional groups in all samples, indicating active sites for hydrocarbon adsorption. The study demonstrates that biochars- particularly RHB and CHB- are promising adsorbents for hydrocarbon remediation, offering dual benefits of pollutant removal and carbon sequestration in soils. The unique composition of CD may enhance soil restoration by contributing essential nutrients. Future studies will evaluate adsorption efficiencies, long-term carbon retention and potential synergistic application of these materials for sustainable soil restoration and carbon capture strategies.

Keywords: pollutant adsorption, graphite, chaoite, carbon capture, environmental cleanup

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MULTIFUNCTIONAL SIGNAL TRACER-MEDIATED IMMUNOSENSORS: RATIONAL DESIGNS AND SENSING APPLICATIONS

Dan Chang^a, Jianyang Feng^a, Chuan Dong^a, Shaomin Shuang^{a*}

^aShanxi University, PR China

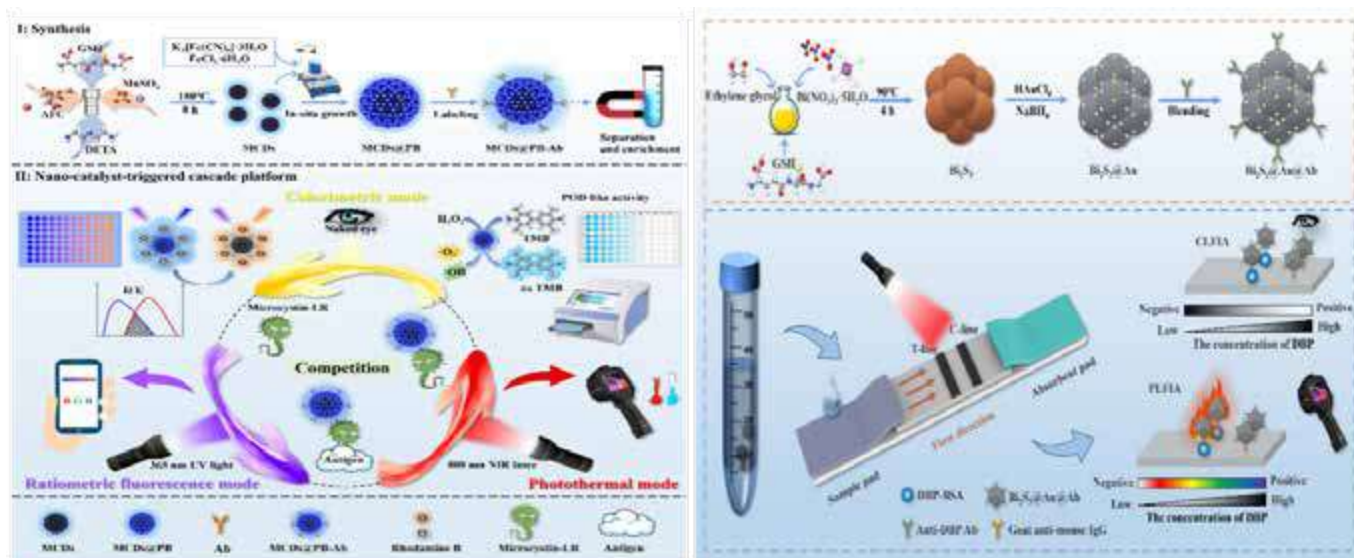
*Corresponding author: smshuang@sxu.edu.cn

Abstract

Immunoassays, such as enzyme-linked immunoassay (ELISA) and lateral flow immunoassay (LFIA) have gained considerable attentions in disease diagnosis, food safety, and environmental monitoring¹. However, conventional single-mode colorimetric methods are vulnerable to external interference, leading to compromises in sensitivity and accuracy². To ameliorate these defects, designing an ideal multifunctional signal tracer is the key to advance high-performance immunoassays and expand its application range.

Our group has conducted researches on multifunctional signal tracer-mediated immunosensors. By incorporating diverse functional nanomaterials into a platform to construct nanocomposites, multifunctional signal tracer-mediated biosensors greatly acquire improvement. (1) A “Three-in-One” multifunctional nanohybrids ($\text{Fe}_3\text{O}_4@\text{MCDs}@\text{PB}$) are designed by employing magnetic carbon dots ($\text{Fe}_3\text{O}_4@\text{CDs}$) coupled with in-situ growth of Prussian blue (PB) and integrated into ELISA platform for powerful magnetic separation/enrichment and colorimetric/ratiometric fluorescence/photothermal multimodal detection of Microcystin-LR. (2) Considering the photothermal property of Bi_2S_3 and high antibody affinity of gold nanoparticles (AuNPs), spark-type $\text{Bi}_2\text{S}_3@\text{Au}$ nanoflowers are used to establish colorimetric/photothermal dual-mode LFIA for point-of-care testing of dibutyl phthalate. Hence, these novel immunosensors preserve the simplicity of colorimetric mode while incorporating quantitative modes of varying sensitivities, which can meet the detection requirements of diverse scenarios and have broad prospects in practical applications.

Keywords: Immunoassays; multifunctional signal tracer; ELISA; LFIA.



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ENHANCED HEPATIC METABOLIC PERTURBATION OF POLYSTYRENE NANOPLASTICS BY UV IRRADIATION-INDUCED HYDROXYL RADICAL GENERATION

Peili Huang^{a*}, Juan Li^b

^aCapital Medical University

^bJilin University

*Corresponding author: huangpl@ccmu.edu.cn

Abstract

The environmental behavior of and risks associated with nanoplastics (NPs) have attracted considerable attention¹. However, compared to pristine NPs, environmental factors such as ultraviolet (UV) irradiation that lead to changes in the toxicity of NPs have rarely been studied². We evaluated the changes in morphology and physicochemical properties of polystyrene (PS) NPs before and after UV irradiation, and compared their hepatotoxicity in mice. The results showed that UV irradiation caused particle size reduction and increased the carbonyl index (CI) and negative charge on the particle surface. UV-aged PS NPs (aPS NPs) could induce the generation of hydroxyl radicals ($\cdot\text{OH}$), but also further promoted the generation of $\cdot\text{OH}$ in the Fenton reaction system. Hepatic pathological damage was more severe in mice exposed to aPS NPs, accompanied by a large number of vacuoles and hepatocyte balloon-like changes and more marked perturbations in blood glucose and serum lipoprotein, alanine aminotransferase and aspartate aminotransferase levels. In addition, exposure to PS NPs and aPS NPs, especially aPS NPs, triggered oxidative stress and significantly damaged the antioxidant capacity of mice liver. Compared with PS NPs, exposure to aPS NPs increased the number of altered metabolites in hepatic and corresponding metabolic pathways, especially glutathione metabolism. Our research suggests that UV irradiation can disrupt the redox balance in organisms by promoting the production of $\cdot\text{OH}$, enhancing PS NPs-induced liver damage and metabolic disorders³. This study will help us understand the health risks of NPs and to avoid underestimation of the risks of NPs in nature.

Keywords: polystyrene nanoplastics, ultraviolet-aged nanoplastics, metabolic pathway, metabolomics, hydroxyl radical.

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EFFECT OF SUPERCRITICAL SOLVENT MEDIA ON THE DEOXYGENATION OF PALMITIC ACID OVER NI-BASED CATALYST

Wajahat Waheed Kazmi*, Faysal M. Al-Khulaifi

^aInterdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

**Corresponding author: wajahat.kazmi@kfupm.edu.sa*

Abstract

Lipid-rich biomass, such as pyrolysis oil derived from spent coffee grounds, contains substantial quantities of triglycerides, which contribute to the formation of free fatty acids in bio-crude. The presence of these oxygenated compounds (comprising approximately 5–20 wt%) complicates transportation and storage while diminishing the calorific value of the resulting fuel. To facilitate the production of clean liquid fuels, the efficient removal of oxygen heteroatoms is a critical and essential step. In this study, palmitic acid was selected as a model compound to represent fatty acids, enabling a comprehensive understanding of the deoxygenation reaction mechanism under supercritical conditions. The upgrading of palmitic acid was conducted in various supercritical solvents using a Ni/activated charcoal catalyst, without the addition of an external hydrogen source. The primary objective was to produce a fuel with lower oxygen content, an improved acid value, and an enhanced heating value. The study systematically investigates the influence of various solvents on product yield and the quality of upgraded oils, alongside catalyst characterization. During the catalytic upgrading process, several reactions—including esterification, hydrogenation, decarbonylation, and decarboxylation—occurred simultaneously. Catalyst characterization was performed using Transmission Electron Microscopy (TEM), N₂-physisorption, and X-ray Diffraction (XRD), while reaction products were analyzed via Gas Chromatography (GC), Gas Chromatography–Mass Spectrometry (GC-MS), and elemental analysis.

Keywords: Palmitic acid, Deoxygenation, Supercritical solvents, Upgrading, Hydrocarbon



Graphic. Upgrading of model compound of bio-oil from waste coffee grounds over Ni based activated charcoal in supercritical solvent

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COSTS AND HUMAN HEALTH EFFECTS OF DEPLOYING CARBON CAPTURE AND STORAGE IN THE US ELECTRIC POWER SECTOR

Wilson H. McNeil^{a,*}, Chelsea Preble^a, Robert Harley^a, Corinne D. Scown^{b,c},

^a*Department of Civil and Environmental Engineering, University of California, Berkeley; Berkeley, CA 94720, USA.*

^b*Life-Cycle, Economics and Agronomy Division, Joint BioEnergy Institute; Emeryville, CA 94608, USA.*

^c*Energy and Biosciences Institute, University of California, Berkeley; Berkeley, CA 94720, USA.*

**Corresponding author: wilsonhm18@gmail.com*

Abstract

Fossil fuels supply most of the energy for electricity generation in the U.S., leading to carbon dioxide (CO₂) emissions and human health effects. Post-combustion carbon capture and storage (CCS) is one method of reducing CO₂ from coal and natural gas combined cycle (NGCC) plants. There can be human health co-benefits of CCS from pre-treating the flue gas for air pollutants to prevent solvent losses. We conducted a cost-benefit analysis of large-scale post-combustion carbon capture and storage adoption in the U.S. considering private costs, monetized CO₂ reduction benefits, and health effects. The minimum criteria used to select applicable plants for retrofit has a direct effect on the quantity of CO₂ emissions that can be reduced through CCS. 97% of CO₂ emissions are potentially addressable through CCS from NGCC plants compared to only 27% from coal plants. Some power plants can have human health benefits with a CCS retrofit, however, we find that many plants would result in a noticeable increase in premature mortality due to increased ammonia (NH₃) emissions from solvent degradation. The social cost of carbon value used affects whether the societal benefits of CCS outweigh the private costs. CCS can contribute to decarbonization goals and can have health co-benefits or co-burdens.

Keywords: carbon capture and storage, air pollution, decarbonization

SACCHAROMYCES CEREVISIAE IMMOBILIZED ZIRCONIUM MODIFIED CELLULOSE FOR PHOSPHATE SEQUESTRATION FROM WATER

R. Parvathi^a, K. Krishna Priyanka^a, M. Christina Nilavu^a, Satyapaul A. Singh^b,
 Vidya Rajesh^{c*}, N. Rajesh^{a*}

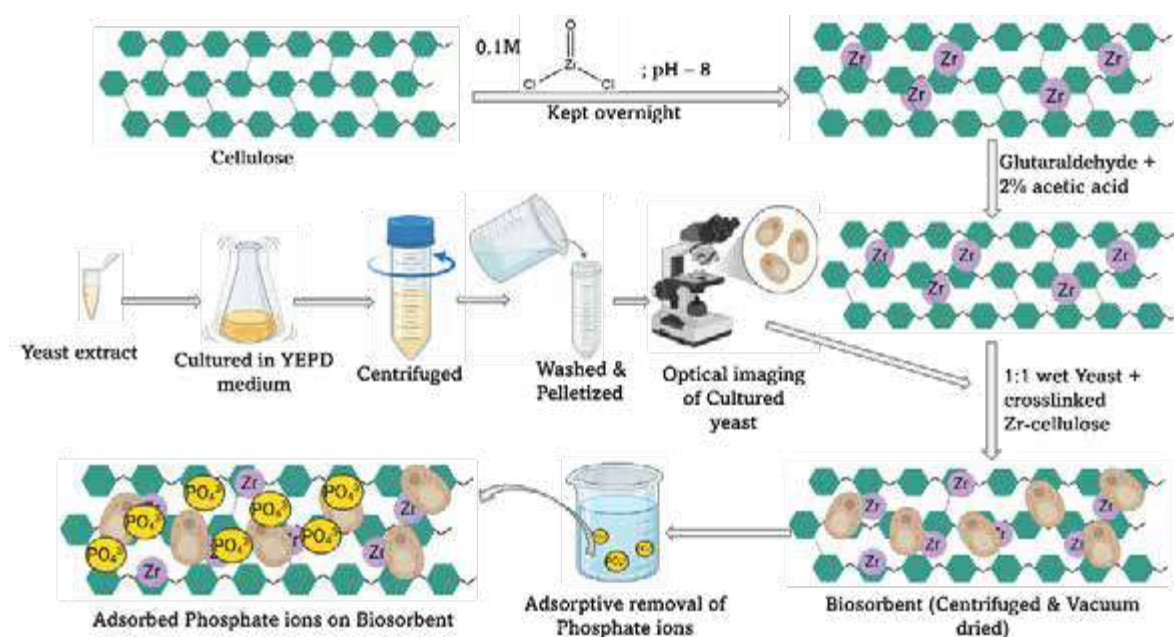
^aDepartment of Chemistry, ^bDepartment of Chemical Engineering, ^cDepartment of Biological Sciences,
 Birla Institute of Technology and Science, Pilani, Hyderabad Campus, Jawahar Nagar, Kapra Mandal,
 Medchal Distict, Telangana 500078, India.

*Corresponding authors: nrajesh@hyderabad.bits-pilani.ac.in; vidya@hyderabad.bits-pilani.ac.in

Abstract

The discharge of surplus phosphate in water results in eutrophication, thereby reducing dissolved oxygen and threatening aquatic ecosystems. Along with natural sources, major contributors to phosphate contamination include agricultural runoff and untreated sewage from households and industries, particularly from fertilizer and laundry wastewater¹. Adsorptive removal of phosphate offers a sustainable solution over the conventional methods such as chemical precipitation, ion exchange owing to its economic feasibility and reusable nature of adsorbents. This study focuses on synthesis of a novel microbial biopolymer composite through a facile method using zirconium impregnated cellulose (Zr-Cellulose) and *Saccharomyces cerevisiae* for phosphate adsorption². The synergistic effect of immobilization significantly enhances the adsorption efficiency for phosphate removal compared to the individual components, as quantified using UV-Vis spectroscopy. Isotherm, kinetic, and thermodynamic studies supports the mechanistic interaction of adsorption. Both the microbe biopolymer composite and Zr-cellulose were characterized through FT-IR, XRF, TGA, SEM-EDS XRD and XPS analysis.

Keywords: biosorbent, *Saccharomyces cerevisiae*, adsorption, phosphate, sustainability



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SYNTHESIS, CHARACTERIZATION, CORROSION INHIBITION, AND MECHANISTIC STUDIES OF NITROBENZALDEHYDE MELDRUM'S ACID IN 1M HCl

Nur Aiman Najwa Kamarul Baharin¹, Sheikh Ahmad Izaddin Sheikh Mohd Ghazali^{1,2}, Fazira Ilyana Abdul Razak, Suhaila Sapari³, Nur Nadia Dzulkifli^{1,2*}

¹School of Chemistry and Environment, Faculty of Applied Sciences, Universiti Teknologi MARA Cawangan Negeri Sembilan, Kampus Kuala Pilah, Pekan Parit Tinggi, 72000 Kuala Pilah, Negeri Sembilan, Malaysia

²Material, Inorganic, and Oleochemistry (MaterInOleo) Research Group, School of Chemistry and Environment, Faculty of Applied Sciences, Universiti Teknologi MARA Cawangan Negeri Sembilan, Kampus Kuala Pilah, Pekan Parit Tinggi, 72000 Kuala Pilah, Negeri Sembilan, Malaysia

³Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 Johor Bahru, Malaysia

*Corresponding author: nurnadia@uitm.edu.my

Abstract

Nitrobenzaldehyde Meldrum's acid (NitroMA) was successfully synthesized and extensively characterized through methods such as elemental analysis, FTIR, and NMR. NitroMA exhibited significant efficacy as a corrosion inhibitor in 1 M HCl, achieving an inhibition efficiency of 82.03 % at an optimal concentration of 0.1 mM. The Langmuir isotherm demonstrated the most accurate fit, with a regression coefficient (R^2) of 0.9989 and a slope of 1.19, effectively representing the adsorption behavior of monolayer adsorbents. NitroMA functions as a mixed inhibitor on the mild steel surface in 1M HCl, engaging in both physisorption and chemisorption interactions, as indicated by the adsorption free energy (ΔG_{ads}) value of $-37.72 \text{ kJ mol}^{-1}$. The formation of a protective barrier that restricts charge transfer and the diffusion of reactive species at the interface between the mild steel and the HCl solution is evidenced by the widening of the semicircle in the Nyquist plots, accompanied by an increase in charge transfer resistance. Higher concentrations of NitroMA inhibitors likely lead to the development of more substantial protective layers on active sites, as reflected by the elevated R_{ct} values, which signify enhanced corrosion inhibition efficiency. As the concentration of NitroMA increases from 0.02 to 0.1 mM, the corrosion rate decreases from 1.3105 mm/year to 1.0827 mm/year, while the corrosion current density (I_{corr}) experiences a significant reduction. NitroMA functions as a mixed-type inhibitor, primarily controlling the cathodic process. The SEM-EDX and AFM images reveal a smoother mild steel surface at a concentration of 0.1 mM NitroMA. Overall, the combined experimental and computational (DFT and Mulliken charge) results confirm NitroMA's effectiveness as a corrosion inhibitor for mild steel in acidic environments, highlighting its ability to absorb onto the surface through a dual mechanism of physisorption and chemisorption.

Keywords: Meldrum's acid, corrosion, DFT, AFM, Mulliken charge

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NITRITE DETERMINATION IN WATER SAMPLES BASED ON ELECTROCHEMICAL METHOD USING DIAZOTIZATION COUPLING REACTION WITH CEFIXIME

S. Georgieva^{a,*}, A. Bezfamilnyi^a, Petar Todorov^b

^aDepartment of Analytical Chemistry, University of Chemical Technology and Metallurgy, st. Kliment Ohridski 8, Sofia, Bulgaria 1756

^bDepartment of Organic Chemistry, University of Chemical Technology and Metallurgy, st. Kliment Ohridski 8, Sofia, Bulgaria 1756

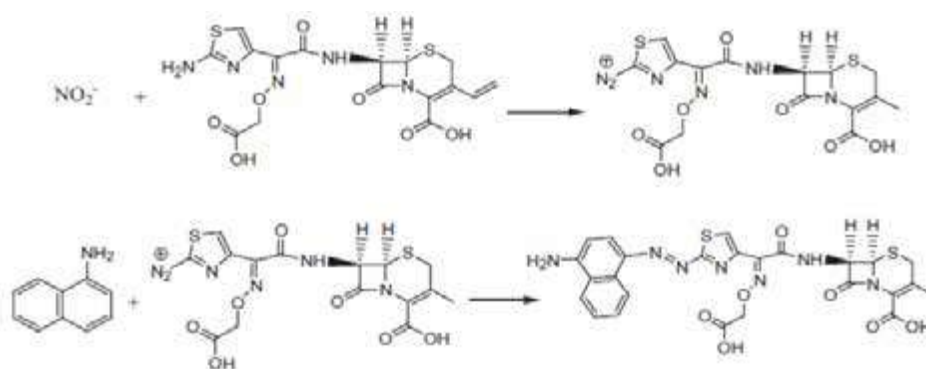
*Corresponding author: st.georgieva@uctm.edu

Abstract

To develop an electrochemical method for the determination of nitrite ions in surface waters, the possibility of a diazotization-coupling reaction between nitrite, cefixime and 1-naphthylamine in an acidic medium was investigated. The electrochemical behavior of the azo dye obtained by the reaction has been studied using the voltammetric method with glass carbon working electrode (GC), Ag / AgCl, (3 mol / L) KCl reference electrode and carbon auxiliary electrode. The best-formed reduction peak obtained by cleavage of the N = N center of the azo bond was observed in phosphate buffer solution (pH 6.89). Specific voltammetric techniques such as cyclic (CV) and differential pulse polarography (DPP) were applied to determine the nature of the electrode reaction of the resulting azo dye. It was found that the reduction of the azo component is quasi-reversible and the analytical signal increases proportionally both with increasing analyte concentration and with increasing scan rate, which shows that the electrode process is diffusion-controlled. The results obtained were applied to the direct detection of nitrite anions in aqueous samples. The relatively low detection limit and a wide dynamic linear range proved both sensibility of the method and the advantages of the method over the reported ones for the determination of nitrite in different water samples.

Keywords: nitrite determination, cefixime, electrochemistry, water samples

Graphic / Image



Acknowledgements

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DIRECT Z-SCHEME $\text{MoS}_2/\text{Bi}_2\text{O}_2\text{CO}_3$ NANOCOMPOSITE FOR PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE

Kian Mun Lee^{a,*}, Chin Wei Lai^a, Mohd Rafie Johan^a, Joon Ching Juan^a

^aNanotechnology & Catalysis Research Centre (NANOCAT), Universiti Malaya.

*Corresponding author: leekianmun@um.edu.my

Abstract

Semiconductor photocatalysis is an environmentally friendly technology used for removing various organic pollutants from water¹. The release of huge amounts of dye effluents after the dyeing process from the textile industries harms the aquatic environment because most of these dyes are non-biodegradable and toxic². In recent years, the visible-active MoS_2 photocatalyst has gained particular interest due to its tunable band gaps, which can be adjusted by varying the layer thickness and applied stress, thereby enabling the acquisition of optical absorption under desired light sources³. However, the availability of its surface-active sites for photocatalytic activity is greatly reduced due to its limitation in exposing edge sites. In this work, a series of $\text{Bi}_2\text{O}_2\text{CO}_3$ (BOC) photocatalysts coupled with interlayer-expanded MoS_2 (IEM) were synthesized via a facile two-pot hydrothermal technique. Among all the samples, 5% BOC-IEM nanocomposite exhibited the highest photodegradation with 94% ($4.97 \times 10^{-2} \text{ min}^{-1}$) for Methylene Blue (MB) dye removal under 1 W LED visible light. The performance of 5% BOC-IEM is 1.5 times and 13.4 times higher than that of the parent IEM and BOC, respectively. The outstanding photocatalytic efficiency of 5% BOC-IEM was due to the presence of oxygen vacancies, enhanced light absorption, and improved migration and separation of charge carriers. An Ohmic contact formed at the interfaces of BOC and IEM enhances the Z-scheme charge transfer mechanism, significantly improving the photocatalytic activity of 5% BOC-IEM. Moreover, the 5% BOC-IEM photocatalyst retains high photocatalytic activity even after five consecutive cycles, with a decline of less than 10%.

Keywords: Z-scheme mechanism, interlayer expanded MoS_2 , heterojunction, LED light, Methylene Blue

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THE LIGAND CONJUGATION/ELECTRON-DONATING EFFECT ON CU(I) ELEVATES THE CONVERSION OF CARBON DIOXIDE TO ETHYLENE

Youchao Song^a, Yiwei Zhang^{a*}

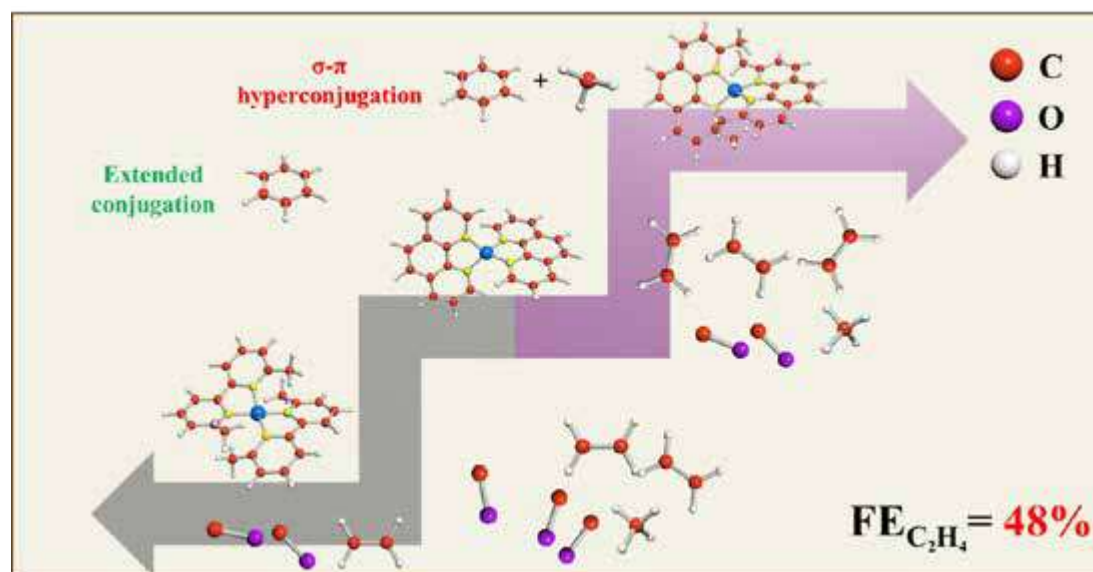
^a*School of Chemistry and Chemical Engineering, Southeast University, Nanjing*

**Corresponding authors: woshizhudadan@163.com*

Abstract

Copper-based molecular catalysts are widely tunable for electrocatalytic CO₂ reduction reactions (CO₂RR) due to their flexible molecular structures. However, the impact of copper's valence state on catalytic performance remains unclear. In this work, we introduced methyl groups into bipyridine/phenanthroline ligands to enhance their electron-donating ability, thereby increasing the proportion of Cu(I) in the catalyst. This adjustment significantly boosted ethylene production. Through in situ electrochemical infrared spectroscopy and density functional theory (DFT) calculations, we found that a higher Cu(I) content lowered the energy barrier for the key step of converting 2*CO to *OCCO, leading to an increased concentration of the *OCCO intermediate. This research demonstrates a new strategy for controlling the electronic environment of the central metal atom via ligand modifications, paving the way for the development of more efficient molecular catalysts with tailored product selectivity.

Keywords: Copper-based molecular catalysts, electrocatalytic CO₂ reduction reactions, bipyridine/phenanthroline ligands, electron-donating, ethylene production



POLYBUTYLENE TEREPHTHALATE-DERIVED METAL-ORGANIC FRAMEWORKS AS ADSORBENTS FOR WATER PURIFICATION

Hiroki Konno^{a*}, Koki Satoh^a, Shintaro Iwaya^a, Momoka Someya^a

^aToho University

*Corresponding author: hiroki.konno@sci.toho-u.ac.jp

Abstract

Metal-organic frameworks (MOFs) have attracted significant interest as advanced molecular-separation materials with application prospects in gas separation, molecular storage, solid catalysts, drug delivery systems, and water treatment. Among them, MIL-53(Al) and UiO-66(Zr) frameworks can be synthesized by numerous methods using polyethylene terephthalate (PET) as the starting material¹, and this promotes the recycling rate of PET. However, poly(butylene terephthalate) (PBT), which is a widely utilized disposable one-way engineering plastic in construction and automotive industries, can also be deployed as a starting material to promote recycling. Thus, the one-pot synthesis of MIL-53(Al) and UiO-66(Zr) was explored using PBT as the starting material.

In this study, we explored the PBT-, PBT with glass fiber (PBT/GF)-, 1,4-benzenedicarboxylate (BDC) reagent-, and PET-derived MIL-53(Al) and UiO-66(Zr) as BDC sources for synthesizing MOFs. Briefly, MIL-53(Al) was synthesized by a one-pot hydrothermal synthesis, and UiO-66(Zr) was synthesized by a one-pot solvothermal synthesis in acetone with hydrochloric acid². The results revealed that the obtained PBT-derived MOFs exhibited high crystallinity that was comparable to those of the BDC reagent-derived MOFs even when glass fiber-blended PBT was used. Thereafter, the high crystallinity PBT-derived MIL-53(Al) and UiO-66(Zr) were deployed as liquid-phase adsorbents for removing metronidazole and benzophenone-4, which are significant constituents of recently reported water contaminants, respectively, demonstrating high adsorption performance, similar to those of BDC-derived MOFs. Additionally, their adsorption isotherms followed the Langmuir model, indicating that the inner parts of their micropores acted as adsorption sites.

This synthesis process could serve as a basis for upcycling waste PBT into effective adsorbents. Moreover, these PBT-derived MIL-53(Al) and UiO-66(Zr) functioned as effective liquid-phase adsorbents for removing contaminants from water.

Keywords: metal-organic frameworks, waste utilization, water purification, adsorption

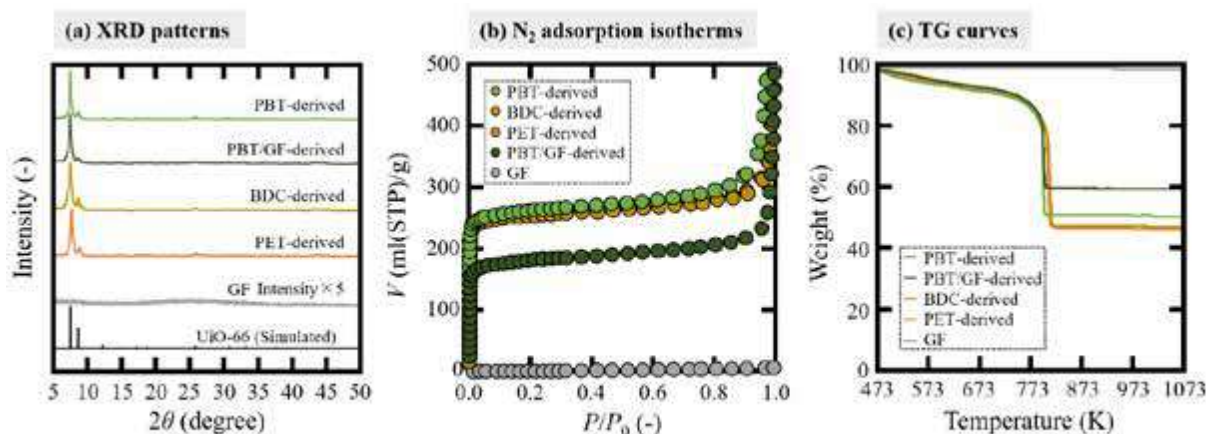


Fig. Characterizations of PBT-derived UiO-66(Zr) Framework

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SUSTAINABLE SYNTHESIS OF FUNCTIONALISED CARBON QUANTUM DOTS FOR COPPER ION DETECTION

Tong Ling Tan^{a,*}, Jia Syuen Chuah^a, Jun Jie Lai^a, See Wei Yong^a, Suraya Abdul Rashid^b

^a Department of Pharmaceutical Chemistry, School of Pharmacy, IMU, Bandar Bukit Jalil, 57000 Kuala Lumpur, Malaysia

^b Institute of Nanoscience and Nanotechnology, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

*Corresponding author: TongLingTan@imu.edu.my

Abstract

The increasing contamination of water sources with heavy metal ions, particularly copper (Cu^{2+}), poses a significant threat to environmental and public health due to their toxicity and bioaccumulation potential. Conventional methods for copper detection often require expensive instrumentation, complex procedures, and generate secondary pollution. To address this, the present study focuses on the sustainable facile synthesis of functionalized carbon quantum dots (N-CQDs) as a low-cost, eco-friendly, and efficient alternative for Cu^{2+} ion detection in aqueous systems. Functionalized CQDs were synthesized via a one-step green microwave method using an empty fruit bunch biochar as a carbon precursor and urea as a nitrogen source, ensuring minimal environmental footprint. The morphological, optical and surface properties of N-CQDs were characterized using TEM, FTIR and PL analysis. TEM images showed uniformly dispersed, spherical particles with diameters ranging from 2–5 nm. FTIR analysis confirmed the presence of hydroxyl, carboxyl, and amine functionalities, which facilitate metal ion binding. The resulting N-CQDs exhibited strong photoluminescence and demonstrated a rapid and sensitive fluorescence quenching response in the presence of Cu^{2+} ions, enabling efficient detection at low concentrations. The sensing detection of Cu^{2+} was performed through visual analysis of the color change and the intensity of the emission peaks. The fluorescence quenching of N-CQDs at 325 nm excitation wavelength could be quenched by adding Cu^{2+} , due to the dynamic quenching mechanism, which showed higher sensitivity to Cu^{2+} in the range of 50–500 nM. This work not only advances the sustainable synthesis of nanomaterials but also contributes to the development of eco-friendly and cost-effective nano sensors for heavy metal ion detection in the real-world sensing applications.

Keywords: Carbon quantum dots; nitrogen; copper; detection; fluorescence

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COMPARISON BETWEEN SINGLE-CHAMBER AND DUAL-CHAMBER PHOTOCATALYTIC FUEL CELL ON SYNTHETIC DYE REMOVAL EFFICIENCY AND POWER GENERATION

Jia Chee Liu, Antonio Choon Kiat Anak Niang, Meng Guan Tay*

Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia

**Corresponding author: mgtay@unimas.my*

Abstract

Photocatalytic fuel cell (PFC) is the combination of photocatalysis and fuel cell that can be used to treat wastewater and produce electrical energy simultaneously. Dual-chamber photocatalytic fuel cell (DCPFC) has been reported to have better performance than single-chamber photocatalytic fuel cell (SCPFC) because of the ability to prevent the electron-hole recombination in DCPFC. But there was not many side-by-side studies found in the literature to compare the performance in between SCPFC and DCPFC. This study presents a comprehensive comparison at different parameter between typical SCPFC and DCPFC for the synthetic methyl red dye degradation and power generation under different conditions. The performance of PFC influenced by the electron transfer driven by potential difference between two electrodes. SCPFC system suffers from the fast recombination of electron-hole pairs. In the present study, a DCPFC setup was setup by separating the photoanode and cathode into two different chambers to prevent the rapid electron-hole recombination. Both types of PFC used ZnO/Zn as photoanode to treat the 10 ppm synthetic methyl red dye solution at pH 4. The DCPFC achieved a highest power generation (130.24 mW/cm²) and 100% dye degradation, significantly outperforming than SCPFC which obtained the highest power generation (59.85 mW/cm²) and 12.23% dye degradation. The ZnO/Zn photoanode can be reused twice in DCPFC but only once in SCPFC. This study highlights the advantages of DCPFC in its' performance and hence the design can be served as a model for the future reference. Indeed, the output of the research aligns with SDGs in clean water, clean energy, and life below water.

REVOLUTIONIZED QUANTUM EFFICIENCY OF GRAPHENE OXIDE BASED COMPOSITES FOR ORGANIC POLLUTANTS REMEDIATION

Siti Nor Atika Baharin^{a,*}, Syafarina Farisa Sateria^a, Zulhatiqah Zolekafeli^a,
Ahmad Husaini Mohamed^a and Kavirajaa Pandian Sambasevam^{a,b}

^a*School of Chemistry and Environment, Faculty of Applied Sciences, Universiti Teknologi MARA,
Cawangan Negeri Sembilan, Kampus Kuala Pilah, 72000 Kuala Pilah, Malaysia*

^b*Electrochemical Material and Sensor (EMas) Group, Universiti Teknologi MARA, 40450 Shah Alam, Selangor,
Malaysia*

*Corresponding author: atikabaharin@uitm.edu.my

Abstract

In this work, an eco-efficient photocatalyst of graphene oxide-based composites with semiconductor materials such as molybdenum disulfide and tungsten disulfide were studied for photocatalytic degradation of organic pollutants. In environmental remediation, graphene oxide (GO) and its composites have become ground-breaking materials, especially for the photocatalytic removal of organic contaminants from water. This work highlights the higher photocatalytic activity of graphene oxide-based composites under visible light irradiation and investigates their increased quantum efficiency. When other nanomaterials are added, the special qualities of graphene oxide (GO), like its large surface area, adjustable surface chemistry, and remarkable adsorption ability, are enhanced even more. Intensive physicochemical properties of the composites were evaluated with FTIR, X-ray diffraction, UV-Visible with Tauc plot analysis, FESEM and surface area analysis. Better light absorption, effective electron-hole separation, and a rise in reactive oxygen species (ROS) are the outcomes of this combination and were evaluated via photoluminescence and electron impedance study. The composites' energy band structure is optimized to minimize electron-hole recombination and maximize photocatalytic degradation rates, which indicate the improved quantum efficiency. These elements support the efficient and quick breakdown of perfluorinated compounds, antibiotics, and other persistent organic pollutants. The results show that GO-based composites are a viable option for next-generation sustainable water filtration technologies, providing an environmentally remediable scalable solution.

Keywords: Graphene Oxide; Nanocomposite; Photocatalysis; Semiconductor Materials

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HIGHLY EFFICIENT DYE REMOVAL FROM WASTEWATER USING BANANA STEM ACTIVATED CARBON AND ALUM IN A SYNERGISTIC ADSORPTION–COAGULATION SYSTEM

Anis Syazwani Salimi^a, Marina Mokhtar^{b,*}, Norain Isa^a, Nur Fadzeelah Abu Kassim^a
Nor Aziyah Bakhari^b

^a Faculty of Chemical Engineering, Universiti Teknologi MARA Cawangan Pulau Pinang, 13500 Permatang Pauh, Penang, Malaysia

^b Department of Applied Sciences, Universiti Teknologi MARA Cawangan Pulau Pinang, 13500 Permatang Pauh, Penang, Malaysia.

*Corresponding author: mmarina@uitm.edu.my

Abstract

Standalone adsorption or coagulation methods for removing methylene blue are often inadequate for fully eliminating dissolved dyes and tend to produce large amounts of sludge, posing disposal and environmental challenges. Therefore, this study explores the efficacy of a combined adsorption–coagulation system for the removal of methylene blue from aqueous solutions, utilizing activated carbon derived from banana stem (ACBS) in conjunction with alum as the coagulant. The ACBS was characterized via Brunauer–Emmett–Teller (BET) and Fourier-transform infrared spectroscopy (FTIR), revealing a high specific surface area of 861.82 m²/g, a pore volume of 0.9872 m³/g, and the presence of surface functional groups favorable for adsorption interactions. Adsorption equilibrium was best described by the Langmuir isotherm model, suggesting monolayer adsorption on a homogenous surface, while the kinetics conformed to the pseudo-second-order model, indicating chemisorption as the dominant mechanism. Optimization studies demonstrated that increasing the dosages of ACBS and alum synergistically enhanced dye removal efficiency, achieving up to 99.92% removal. These results validate the potential of ACBS–alum as an efficient, sustainable, and low-cost system for dye-laden wastewater treatment. Notable limitations include potential experimental inaccuracies due to equipment calibration frequency and procedural reproducibility.

Keywords: activated carbon, banana stem, adsorption–coagulation, methylene blue, kinetics



Banana stem waste

→
Activation and pyrolysis



Activated Carbon Banana Stem (ACBS)

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PHYTOCHEMICAL ANALYSIS, ANTIOXIDANT AND ANTIBACTERIAL ACTIVITY OF ECOENZYME SOAP FROM ROCK MELON (*CUCUMIS MELO* L.) PEELS

Wan Zuraida Wan Mohd Zain^{a,b,*}, Nur Sakinah Asya^a, Amyra Hazwani Ghazali^a, Siti Alwani Ariffin^{b,c}, Afiqah Mohammad^c, Neneng Windayani^d

^aFaculty of Plantation and Agrotechnology, Universiti Teknologi MARA, Cawangan Melaka, Kampus Jasin, 77300 Merlimau, Melaka, Malaysia.

^bMarine Pharmaceutical Research Group (MaReG), Puncak Alam Campus University Teknologi MARA (UiTM), 42300 Bandar Puncak Alam, Selangor Darul Ehsan Malaysia.

^cFaculty of Pharmacy, Universiti Teknologi MARA, Cawangan Selangor Kampus Puncak Alam Bandar Puncak Alam, 42300 Puncak Alam, Selangor, Malaysia.

^dDepartment of Master Science Education, Postgraduate, Sunan Gunung Djati State Islamic University, Bandung 40614, Indonesia

*Corresponding author: wanzuraida@uitm.edu.my

Abstract

Cucumis melo var. *cantalupensis* (rock melon) is a tropical fruit valued for its nutritional and phytochemical content. Its peel, a rich source of bioactive compounds, can be valorized through ecoenzyme technology. Ecoenzyme based formulations have gained prominence in the cosmeceutical sector due to their potential to enhance the bioefficacy of natural bioactives, particularly in skincare. This study aimed to evaluate the physicochemical properties, phytochemical constituents, antioxidant capacity, and antimicrobial efficacy of ecoenzyme liquid soaps derived from rock melon peel and whey. Three soap formulations were developed: RE (rock melon extract), ER (rock melon peel ecoenzyme), and ERW (rock melon peel ecoenzyme enriched with whey). Physical properties including pH, foam stability, and organoleptic characteristics were assessed under stability conditions at 23°C and 27°C. Enzymatic profiling (amylase and lipase activity), GC-MS, and phytochemical screening were conducted to identify key bioactive constituents. Antioxidant activity was quantified using the DPPH radical scavenging assay, total phenolic content (TPC), and total flavonoid content (TFC). Antibacterial efficacy was determined using the agar well diffusion method against a panel of Gram-positive and Gram-negative bacteria. Statistical analysis was performed using two-way ANOVA in GraphPad Prism (version 10.4.1). All formulations exhibited slightly acidic pH (5.24–5.75) and high foam stability (82.9–95.12%). GC/MS profiling detected nonpolar compounds including phenolics, flavonoids, terpenoids, and alcohol derivatives (Figures 1–3). Enzyme assays confirmed the presence of amylase and lipase. The ERW formulation demonstrated the most potent antibacterial activity, particularly against *Staphylococcus aureus*, MRSA, *Bacillus cereus*, *Bacillus subtilis*, and *Burkholderia glumae*. ERW also exhibited superior antioxidant properties, with the lowest IC₅₀ (105.05 µg/mL), highest TPC (720.3 mg GAE/g), and TFC (552.9 mg QE/g). Whey-enhanced rockmelon peel ecoenzyme (ERW) significantly enhanced the biofunctional properties of the liquid soap, highlighting ERW as a promising candidate for natural skincare applications with strong antibacterial and antioxidant potential.

Keywords: Rock melon, ecoenzyme, soap, phytochemical screening, GC-MS antioxidant, antibacterial.

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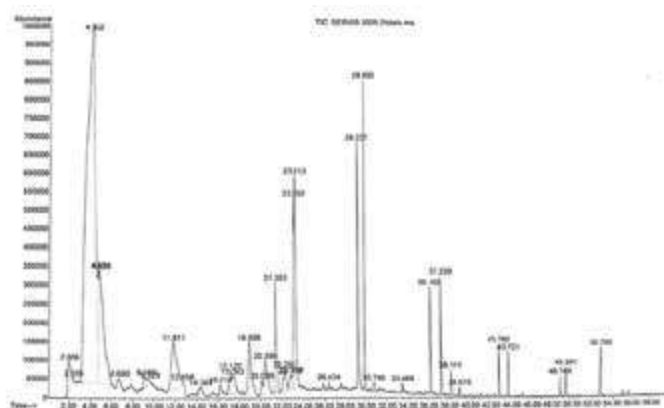


Figure 1. GC-MS chromatograms of ERW

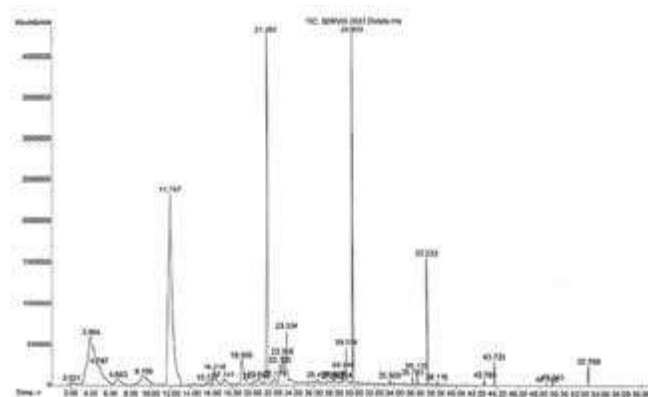


Figure 2. GC-MS chromatograms of ER

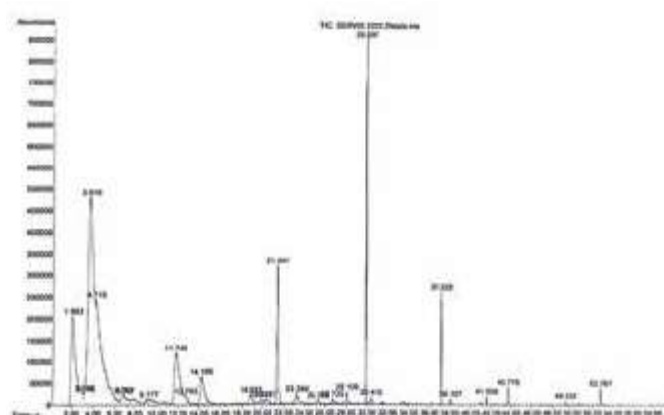


Figure 3. GC-MS chromatograms of RE

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TRAP INLAID CATIONIC HYBRID COMPOSITE MATERIAL FOR EFFICIENT SEGREGATION OF TOXIC CHEMICALS FROM WATER

Sahel Fajal,^a Writakshi Mandal,^a Samraj Mollick,^a Yogeshwer D. More,^a Arun Torris,^b
Satyam Saurabh,^a Mandar M. Shirolkar,^c and Sujit K. Ghosh^{a*}

^aDepartment of Chemistry, and Centre for Water Research, Indian Institute of Science Education and Research,
Dr. Homi Bhabha Road, Pashan, Pune 411008, India.

^bPolymer Science and Engineering Division, CSIR-National Chemical Laboratory,
Dr. Homi Bhabha Road, Pune 411008, India.

^cSymbiosis Center for Nanoscience and Nanotechnology (SCNN) Symbiosis International (Deemed University)
(SIU), Lavale, Pune 412115, India.

*Corresponding author: sghosh@iiserpune.ac.in

Abstract

Oxoanions made of metals are potentially harmful contaminants that seriously pollute the water. As a result, the separation of these species has recently drawn a great deal of research interest. Several excellent adsorbents have been used to manage chemicals effectively, but their restricted microporous nature, non-monolithic applicability, relatively sluggish kinetics, and lower selectivity prevented their widespread real-time use. In this study, we developed an innovative anion exchangeable hybrid composite aerogel material (IPcomp-6), which combines a stable cationic metal-organic polyhedron with a hierarchically porous metal-organic gel that is programmed with specific oxoanions trapping moieties. Even when there was a 100-fold excess of other coexisting anions, the composite scavenger was able to segregate different hazardous oxoanions from water, including, HAsO_4^{2-} , SeO_4^{2-} , ReO_4^- , CrO_4^{2-} , and MnO_4^- . Even at low concentrations and considerably below the As(V) limit for drinking water set by the WHO, the material was able to selectively remove traces of HAsO_4^{2-} . Moreover, the hybrid material can successfully eliminate arsenate from natural drinking water samples and simulated industrial wastewater samples, in both batch and dynamic column exchange sorption experiment. The mechanistic role of multifunctionalities of IPcomp-6 towards efficient arsenate capture was further investigated by numerical flow-velocity experiments along with theoretical calculations.

Keywords: Environmental remediation, Chemical separation, Pollutants capture, Toxic chemicals, Safe water, Porous materials, MOFs

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NEXT GENERATION RISK ASSESSMENT APPLIED TO NANOPESTICIDES

Melanie Kah^{a*}, Rai Kookana^b, Jose Tarazona^c

^aThe University of Auckland, School of Environment, New Zealand

^bUniversity of Adelaide, Waite Campus, Glen Osmond, Australia

^cSpanish National Environmental Health Center. Instituto de Salud Carlos III. Madrid, Spain

*Corresponding author: melanie.kah@auckland.ac.nz

Abstract

The application of nanotechnology to develop and improve pesticides has been the topic of intense research and development activities over the last decade. Current challenges associated with the regulatory risk assessment of nanopesticides are one reason for their slow market uptake, which may be a missed opportunity to improve current agricultural practices. Guiding principles to adapt ecological and human health risk assessments were previously developed through a series of multisectoral workshops involving scientists, regulators, and industry, and supported by the IUPAC [1, 2, 3].

Our latest workshop evaluated the potential application of Next Generation Risk Assessment (NGRA) to nanopesticides. The main drivers for NGRA are the incorporation of molecular, computational and system biology developments in risk assessment, with a focus on animal-free New Approach Methodologies (NAMs). NGRA entails a more mechanistically based risk assessment paradigm and the use of hypotheses, based on this mechanistic understanding and a comprehensive evaluation of exposure potential. NGRA is an emerging approach that is particularly relevant for assessments at the nano-scale.

In this presentation, we will illustrate how NGRA can be applied to nanopesticides. Several case studies have been selected to illustrate how hypotheses driving the NGRA can be established on the basis of three main information sources: (1) the expected exposure pathway for each human group or ecological taxa, (2) the previous knowledge on toxicity of the active substance and relevant co-formulants, and (3) the characteristics and benefits expected by the nano design of the plant protection product. We hope that the proposed framework can serve as a foundation to advance the risk assessment of nanopesticides as well as other advanced materials that do not easily fit in with existing approaches.

Keywords: nanopesticides, nanofertilisers, nanocarriers, risk assessment

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NOVEL MINERAL-HYDROGEL COMPOSITES FOR SUSTAINABLE NUTRIENT RECOVERY AND DELIVERY

Young-Shin Jun^{a*}, Minkyung Jung^a, Albern X. Tan^a

*^aDepartment of Energy, Environmental & Chemical Engineering, Washington University,
St. Louis, MO 63130, USA*

**Corresponding author: ysjun@wustl.edu*

Abstract

Unbalanced nutrient management of phosphorus (P) and nitrogen (N) leads to harmful algal blooms (HABs), threatening industries such as fisheries and tourism, and posing public health risks through cyanobacterial toxin production. Ironically, there is a critical global shortage of phosphorus resources. To simultaneously address these issues and promote environmental sustainability, we developed novel calcium alginate hydrogel composites embedded with nanosized minerals to effectively remove and recover P and N from wastewater. These composites can subsequently be used as nutrients/fertilizers in biorefinery or agricultural practices.

In this invited talk, I will discuss an innovative nutrient removal and recovery method that employs calcium alginate (Ca-Alg) and calcium phosphate (CaP) mineral seeds to capture P and N from various nutrient-rich wastewaters, especially municipal wastewater. The first type of mineral–hydrogel composite is seeded with calcium phosphate and calcium silicate-based minerals (Ca-Alg/CaP+Wollastonite (CaSiO_3)) to efficiently remove and recover P as phosphate. For the simultaneous removal and recovery of P and N (ammonia), the second type of composite incorporates struvite minerals (Ca-Alg/CaP+Struvite ($\text{NH}_4\text{MgPO}_4 \cdot 6\text{H}_2\text{O}$)). We tested these two types of mineral–hydrogel composites for nutrient recovery from nutrient-rich water and demonstrated their effectiveness in managing HABs. The composites incorporated *in situ*-formed seeds of struvite and CaP, reducing the nucleation energy barrier and enhancing heterogeneous nucleation kinetics even under undersaturation conditions. The unique local chemistry of the mineral–hydrogel composites created by hydrogel encapsulation plays critical roles in promoting the composite performance.

This innovative approach provides a new way to lower nutrient levels before wastewater discharge into streams. Furthermore, encapsulating phosphate and ammonia within the hydrogels offers potential for reuse in agricultural and biorefinery applications. This research highlights a significant advancement in nutrient management technology, addressing both environmental and resource scarcity challenges.

Keywords: Mineral, hydrogel, nucleation, nutrients, phosphate

TAILORED NANOMATERIALS FOR DRUG DELIVERY APPLICATIONS AND THEIR PROSPECTS IN NANO-AGROCHEMICALS USE

Kasturi Muthoosamy^{a,*}, Ayesha Ashraf Khan^b, Asgar Ali^{b,c}

^a*Department of Chemical and Environmental Engineering, University of Nottingham Malaysia, Semenyih, Selangor, Malaysia*

^b*Centre of Excellence for Postharvest Biotechnology (CEPB), School of Biosciences, University of Nottingham Malaysia, Semenyih, Selangor, Malaysia*

^c*The UWA Institute of Agriculture, The University of Western Australia, Perth, Washington, Australia*

*Corresponding author: kasturi.muthoosamy@nottingham.edu.my

Abstract

The integration of nanotechnology in the medical field, specifically in the drug delivery systems has allowed major development in cancer research. Drug delivery can be made nano-sized with various advantages such as higher potency, enhanced efficacy, and lower toxicity, consequently prolonging patient survival. Prior to developing/synthesizing a nanomedicine, several consideration has to be given to its design. Factors such as morphology (size, shape, surface roughness), overall charge, surface area and available functional groups must be carefully considered. The route of administration of nanomedicine and the uptake mechanism, are even more imperative^{1,2}. Adapting these criteria, nano- agrochemicals including nanocoatings can be developed with similar prognosis on plants. The current work looks into the design and development of chitosan-zinc oxide nanoemulsion as anti-bacterial barrier for plants and post-harvest crops. Several methods of synthesis including green chemistry and sonochemistry are explored². The application of chitosan-zinc oxide coatings to papaya demonstrated that coated fruits exhibited a delayed onset of anthracnose disease³ and reduced disease severity compared to non-coated fruits. The findings open up possibilities for smart delivery system in plants which looks into dye- tagged or fluorescent nanomaterials (nanoclusters) for theranostics purposes (imaging, diagnosis and therapy), along with controlled drug release⁴. Such advances in nanomedicine has allowed sustainable, low cost and biodegradable systems with low toxicity which can be translated into the field of nano-agrochemicals for high-value crop production.

Keywords: nanotechnology, nanoemulsion, chitosan-zinc oxide, nano-agrochemicals, nanocoatings

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UNDERSTANDING THE INTERACTIONS OF POLYMER NANOCARRIERS USED IN AGROCHEMICALS USING WATER-LIGAND OBSERVED VIA GRADIENT SPECTROSCOPY (WATER LOGSY) NMR

Dona Manayath^{a,b}, Jadranka Travas-Sejdic^{a,b}, Melanie Kah^{a*}, Erin M. Leitao^{a,b*},

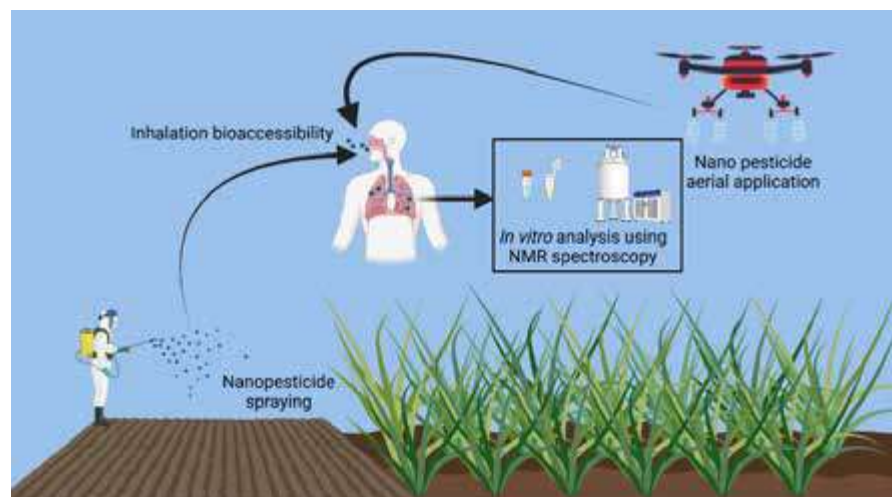
^a The University of Auckland, New Zealand.

^b The MacDiarmid Institute of Advanced Materials and Nanotechnology, New Zealand.

*Corresponding authors: melanie.kah@auckland.ac.nz, erin.leitao@auckland.ac.nz

Abstract

Polymer nanocarriers (PNCs) refer to soft nanoparticles with a high surface-to-volume ratio, favouring surface conjugation with functional moieties such as fluorescent tags, drugs, small molecules, and metals.¹ PNCs have stimulated much interest in recent years due to their versatility and tunability. PNCs can be loaded with cargo, such as an active ingredient (AI) (e.g. drugs, pesticides), during or after their synthesis.² The ability to control the release of the AI from the PNCs and to modify their stimuli-responsive behaviour makes them useful in a wide number of delivery applications³ across various disciplines such as medicine, agriculture, veterinary drugs, cosmetics, and food technology. Water-soluble polymer nanocarriers, such as those based on polyacrylic acid, are often used to deliver agrochemicals. Human exposure to PNCs used in agriculture is a matter of concern as the workers or end users could be unintentionally exposed to the PNCs during the different life cycle stages of the agrochemicals either through inhalation, dermal exposure or ingestion. The biointeractions of PNCs in biological fluids are complex and significantly influence the biological fate of the PNCs.⁴ In our research, we aim to investigate the biophysical interactions of the water-soluble PNCs used in agricultural applications considering the various exposure pathways. To achieve this, we are using a unique combination of analytical techniques like Water LOGSY NMR and Nanoparticle Tracking Analysis (NTA) to detect and characterize PNCs, including their particle size and interaction with different artificial biological fluids. The outcomes of this research will support the development of a risk assessment strategy for ensuring the safety of nano agrochemicals.



Keywords: Polymer nanocarriers, biological interactions, bio-corona, human exposure, artificial biofluids

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PHOTON-PHONON CO-DRIVEN CONVERSION OF CH₄ TO C₂

Junwang Tang

Industrial Catalysis Center, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

Corresponding author: jwtang@tsinghua.edu.cn

Abstract

Solar-driven conversion of carbon-containing sources, eg. CO₂ and CH₄ to valuable chemicals is regarded as a pivotal approach for harnessing solar energy and, more importantly, a highly efficient pathway toward achieving carbon neutrality in chemical synthesis. Our early studies on charge dynamics in inorganic materials reveal that the current low solar conversion efficiency is due to both fast charge recombination and sluggish water oxidation [1,2], thus we developed effective material strategies to overcome these challenges and improve the performance of photocatalysis. Typically, we found that surface junctions can substantially facilitate charge transfer and separation. For instance, the junction composed of C₃N₄ and carbon quantum dots which were synthesised by microwave chemistry represents an unprecedented CO₂ reduction efficiency using water as the sole proton source, leading to CO₂ to methanol with a 100% selectivity [3]. More importantly, we discovered that coupling photons with phonons to co-drive catalytic reactions is significantly more efficient and selective compared to solely relying on photocatalysis, which has been demonstrated in a few scenarios, including methane conversion to formaldehyde on Ru/ZnO [4], methane to C₂H₆ over Au loaded TiO₂ [5] etc, all with extremely high conversion and selectivity. Very recently, we developed a new concept of an intramolecular junction, which is composed of alternate benzene and triazine motifs in CTF polymer. Such structure can facilitate fast charge separation and is characterised by spatially separated reduction and oxidation sites in one molecular unit, thus substantially improving the methane conversion to ethanol and mitigating the overoxidation to CO₂, resulting in an unprecedented ethanol yield and selectivity of 80% operated under ambient condition [6].

Keywords: photon-phonon co-driven catalysis, methane, ethane, ethanol, selectivity

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ELECTROCHEMICAL CONVERSION OF CO₂ USING SINGLE ATOM DECORATED CATALYSTS

Soo Young Kim^{a*}, Sang Hyun Ahn^b, Myoung Hwan Oh^c

^aDepartment of Materials Science and Engineering, Korea University, Seoul, Republic of Korea

^bDepartment of Chemical Engineering, Chung-Ang University, Seoul, Republic of Korea

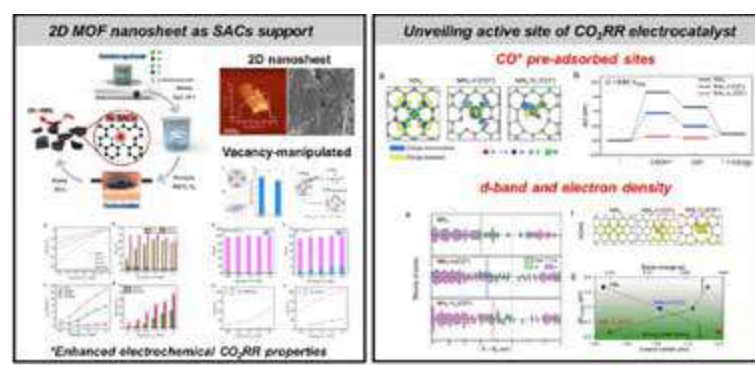
^cDepartment of Energy Engineering, KENTECH, Naju, Republic of Korea.

*Corresponding author: sooyoungkim@korea.ac.kr

Abstract

The pursuit of a circular carbon economy and the need to surmount the constraints of CO₂ electroreduction technology has prompted the development of single-atom catalysts (SACs) for electrocatalysts. SACs consist of isolated metal atoms dispersed on a support material. First, zeolitic imidazolate framework (ZIF)-8 containing various transition metal ions—Ni, Fe, and Cu—at varying concentrations upon doping were fabricated for the electrocatalytic CO₂ reduction reaction (CO₂RR) to CO without further processing. The electron-rich sp² C atoms of optimized copper doping on ZIF-8, leading to a local effect between the Zn–N₄ and Cu–N₄ moieties, achieve a maximum Faradaic efficiency for CO₂ to CO of 88.5% at -1.0 V (vs. RHE) with a stability over 6 h [1]. Second, compared to nanoparticles, SACs have been shown to significantly enhance the efficiency of metal atom utilization by nearly 100%, which results in a higher concentration of active sites, leading to outstanding catalytic activity, excellent product selectivity, and stability. Among the diverse support materials, the ZIFs, a sub-class of metal-organic frameworks (MOFs) with high nitrogen content, have been widely used to prepare metal-nitrogen-doped carbon (M-NC) SACs with dense active sites. Herein, we utilized an eco-friendly approach to produce two-dimensional ZIF-8 nanosheets (ZIF-8-NS) as an optimal support material for SACs. Additionally, we introduced Ni precursor into the synthesis process of Ni-ZIF-8-NS, which was then subjected to pyrolysis at 950 °C under a N₂ atmosphere to yield the final product, Ni-NC-NS. Ni-NC-NS demonstrated an outstanding CO₂ RR performance by exhibiting excellent Faradaic efficiency (FE) toward CO of ~100% both in the H-cell and flow-cell reactors as well as a remarkable turnover frequency (TOF) of 23,699 h⁻¹. [2] Finally, we will present a facile strategy for synthesizing M-NC SACs using metal-chelating ligands, eliminating the need for additional processing steps. Specifically, the method to use ethylenediaminetetraacetic acid as a strong metal-chelating ligand will be shown. [3]

Keywords: Metal-organic framework, CO₂ reduction, Electrocatalysts, Sing-atom catalysts



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PHOTOTHERMAL CATALYSIS FOR REFORMING OF METHANE

Hongqi Sun*, Jinqiang Zhang

School of Molecular Sciences, The University of Western Australia, Perth, WA6009, Australia

**Corresponding author: hongqi.sun@uwa.edu.au*

Abstract

Renewable energies, for example, solar energy has long been contributing to sustaining life and driving natural processes across ecosystems on Earth.[1] Artificial photosynthesis, i.e., photocatalysis, has been demonstrated effective for a range of applications. In recent years, its role has been expanded and strengthened, emerging as a promising alternative to address the pressing challenges of the global energy crisis and climate change. That could innovate conventional thermal catalysis for processing fossil fuels, e.g., dry or steam reforming of methane. However, the solar utilisation efficiency is low, because long wave light of solar heat effect cannot be utilised in photocatalysis. This talk will explore various opportunities for converting solar energy into sustainable fuels and valuable chemicals with full spectrum energy utilisation. By examining materials design, catalytic reactions, and process engineering, we can unlock innovative pathways, for example, photothermal catalysis, for harnessing sunlight in new ways. [2,3] Particular attention will be paid to solar-assisted reforming processes for methane to produce hydrogen or syngas. Additionally, the discussion will highlight how solar energy can serve as a cornerstone for the future of chemical manufacturing, potentially reducing carbon emissions and dependence on fossil fuels. In this way, solar energy stands as a pivotal resource, both for our sustainable future on Earth and for exploring humanity's next frontier.

Keywords: solar energy; photothermal catalysis; reforming; methane; hydrogen

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PHOTOCATALYSIS STUDIED AT SINGLE-PARTICLE LEVEL

Zhaoke Zheng*

State Key Laboratory of Crystal Materials, Shandong University, Jinan, China

*Corresponding author: zkzheng@sdu.edu.cn

Abstract

The real catalytic conversion process exhibits significant surface interface heterogeneity and complex spatiotemporal dynamics at the micro nano scale, requiring high-precision characterization techniques to obtain more accurate surface interface structure-activity relationship information. Single particle fluorescence spectroscopy technology, by monitoring the fluorescence characteristic parameters of individual nanoparticles in situ, can study the specific physical and chemical processes of surface interface structure evolution, charge transfer, and energy transfer at the single particle scale, and can be used to accurately reveal surface interface properties and catalytic mechanisms. In the early stage, we developed a “spatially resolved” single particle fluorescence spectroscopy technology with independent intellectual property rights, and initially achieved the construction of a single particle spectroscopy system with “time-resolved” characteristics. Based on this technology, the transfer of hot electrons from the absorption center to the catalytic center has been confirmed at the single particle level; A microfluidic reaction device was designed to achieve in-situ study of single particle surface reactions under catalytic conditions, revealing the mechanism of carrier driven H_2O molecule activation reaction and non competitive adsorption reaction, and discovering the key role of direct energy transfer mechanism in HCOOH molecule activation; For the first time, nanoscale imaging of BiVO_4 surface defects has been achieved, providing a spatially high-resolution characterization technique for the distribution and imaging of surface defects in solid materials. This has revealed the adsorption and activation mechanism of O_2 molecules by specific active site defects, accelerated interfacial charge transfer, and enhanced the catalytic activity of benzylamine oxidative coupling.

Keywords: single-particle spectroscopy, photocatalysis

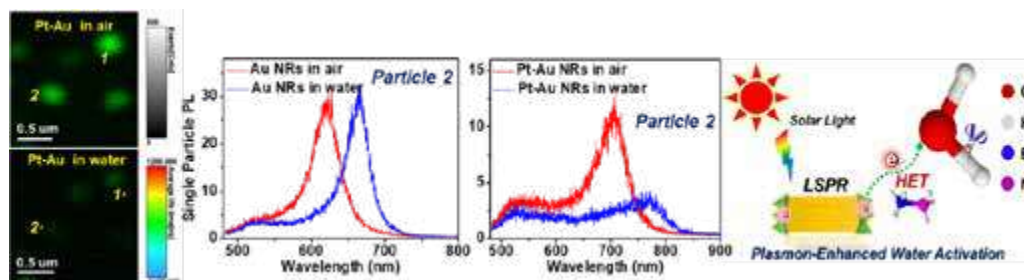


Figure 1: The activation of water molecules by energetic charge carriers

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HETEROGENEOUS MOLECULAR CATALYSIS FOR ELECTROCHEMICAL CO₂ REDUCTION

Yijiao Jiang

School of Engineering, Macquarie University, Sydney, Australia

Email: yijiao.jiang@mq.edu.au

Abstract

Electrochemical reduction of CO₂ in aqueous electrolytes is one of the most promising routes for commercial CO₂ utilization. A switch from the currently used noble metal-based catalysts to the carbon-supported macrocyclic complexes could bring a much-needed cost reduction thus making the technology economically viable. However, the inherently low conductivity and tendency of molecular catalysts to degrade during the long-term operation present a challenge for catalyst design. We applied mechanistic investigations to tackle a challenging problem of the catalyst durability in CO₂ electrolysis. It was determined that the loss of activity takes place due to the reductive carboxylation and co-occurring formation of inactive metal complex. Therefore, the stability could be greatly enhanced through the introduction of bulky donating substituents around the macrocyclic core. These insights allowed us to design and synthesis a catalyst bearing eight methoxy groups around the lateral aromatic moieties which demonstrate an improved stability during the long run electrolysis. These design principles, combined with our recent development of bicarbonate electrolysis and heterogeneous molecular catalysts, would provide a low-cost and very stable catalytic system for CO₂ electrolysis.

Keywords: Heterogenous molecular catalyst, cobalt phthalocyanine, mechanism-driven design, carbon dioxide electroreduction, bicarbonate electrolysis

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CATALYSING SUSTAINABLE CHEMICAL MANUFACTURING

Adam F. Lee^{a,*}

^a*School of Environment and Science, Griffith University, QLD 4222, Australia.*

**Corresponding author: adam.lee@griffith.edu.au; adamfraserlee@gmail.com*

Abstract

The anthropogenic origin of climate change from combustible carbon, and desire to establish a global circular economy is driving the quest for new sustainable manufacturing processes.¹ Catalysis has a rich history of facilitating energy efficient, selective molecular transformations, and will play a pivotal role in overcoming the scientific and engineering barriers to sustainable and economically viable energy vectors and chemicals. This presentation describes challenges in the design of catalytic technologies for biofuels and platform chemicals synthesis.²

Advances in the rational design of nanoporous solid acid and base catalysts enable the fabrication of hierarchical porous architectures³ in which different active sites are spatially compartmentalised. Synergies between nanoporous solid acids and metal nanoparticles organocatalysts also facilitate active and selective upgrading of phenolic components of pyrolysis bio-oils to hydrocarbon fuels, and precious metal thrifting.⁴ Active site compartmentalization and the synthesis of bifunctional organocatalysts (**Figure 1**)⁵ facilitate chemical cascades to produce valuable (bioderived) chemical intermediates.⁶

Keywords: heterogeneous catalysis, biomass, biofuels, chemical cascade

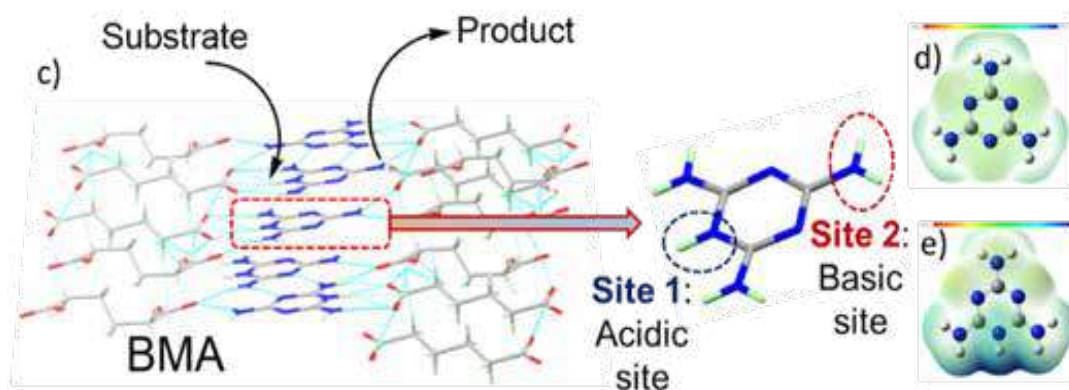


Figure 1. Cascade deacetalisation-Knoevenagel condensation of dimethyl acetals over BMA.

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IN-SITU RAMAN PROBING ELECTROCHEMICAL REACTIONS

Jian-Feng Li^{a,*}

^a*Department of Chemistry, Xiamen University, Xiamen 361005, China*

**Corresponding author: Li@xmu.edu.cn*

Abstract

Understanding the fundamental reaction mechanism and the structure-activity relationship at electro-chemical interfaces is essential for developing electrochemistry and electrocatalysis. Such fundamental understanding is strongly dependent on the surface molecular information of the species at the electro-chemical interfaces, especially those acquired under working conditions. Surface-enhanced Raman spectroscopy (SERS) can provide such information with ultrahigh surface sensitivity. However, only a few metals (like Au, Ag, and Cu) with particular nanostructures can generate strong SERS effects. This material and morphology limitation has greatly hindered the applications of SERS in probing electrochemical reactions.

To overcome the long-standing limitations, we developed various strategies, including the “borrowing” strategy, shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS), and SHINERS-satellite strategy, through the fabrication of plasmonic core-shell nanostructures, allowing in-situ SERS studies at electrochemical interfaces. Using these strategies, the dynamic process of electrocatalytic reactions, such as oxygen reduction reaction (ORR), hydrogen oxidation reaction (HOR), hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and CO₂ reduction reaction (CO₂RR), etc., occurring on model single crystal surfaces or practical nanocatalysts have been systematically investigated. Direct spectroscopic evidence for the key intermediates, such as *OH, *OOH, and *O₂-, as well as interfacial water structure, during reactions has been obtained, which is combined with theoretical simulations to uncover the reaction mechanisms or structure-activity at a molecular level.

Keywords: SERS, in-situ, electrochemistry, interfacial water, reaction intermediates

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CARRIER AND MASS TRANSPORT AT THE ELECTROLYTE INTERFACE

Zheng Liu^{a,*}

^a *Nanyang Technological University, Singapore 639798*

**Corresponding author: z.liu@ntu.edu.sg*

Abstract

Achieving sustainable energy requires advancements in both green energy production and energy efficiency. This presentation addresses carrier and mass transport phenomena at the electrolyte interface to improve the performance of electrocatalysts for sustainable energy conversion.

We first examine the semiconductor-electrolyte interface using two-dimensional (2D) materials as model systems. Conventional Schottky-junction models fail to explain high carrier accumulations in ultrathin semiconductor catalysts. Inspired by ion-controlled electronics, we unveiled a universal “self-gating” phenomenon using in-situ microcell measurements. This clarifies electronic-conduction modulation during electrocatalysis and reveals a surface conductance mechanism: semiconductor type strongly correlates with activity.

Secondly, to address mass transport limitations related to gas evolution at high current densities, we introduce an innovative on-chip microcell-based TIRF platform to investigate nanobubble nucleation dynamics on graphene-supported Pt films. A key strategy involves incorporating interfacial metal layers (IMLs) to regulate bubble nucleation. The introduction of a titanium (Ti) IML triggers delocalized nanobubble evolution (DNE), where nanobubbles form on both the Pt sites and graphene support. DFT calculations show Ti promotes electron transfer, lowering the hydrogen spillover barrier, and facilitating hydrogen migration to the graphene support.

Furthermore, microcell measurements demonstrate enhanced HER for Pt-Ti-graphene, attributed to DNE. These results highlight the significance of carrier transport, mass transport, and novel material designs in developing advanced electrocatalysts for sustainable energy.

Keywords: 2D materials, mass transport, electrolyte interface

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DEFECTIVE LAYERED DOUBLE HYDROXIDE BASED NANOSTRUCTURED PHOTOCATALYSTS FOR NITROGEN FIXATION

Tierui Zhang*

Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 10190, Chin.

**Corresponding author: tierui@mail.ipc.ac.cn*

Abstract

The activation and conversion of nitrogen is one of the most challenging topics in modern chemistry. Industrial nitrogen fixation requires severe reaction conditions of high temperature and high pressure, and at the same time will emit a large amount of greenhouse gases causing serious environmental problems. Photocatalytic nitrogen fixation is considered as a promising artificial nitrogen fixation technology. At present, the performance of photocatalytic nitrogen fixation still needs to be further improved, and it is urgent to develop low-cost and efficient photocatalytic materials. Layered double hydroxide (LDH)-based nanomaterials have attracted much attention due to their advantages of easy structure regulation and simple preparation. In recent years, by creating defect sites on the surface of LDH-based materials, our research group has achieved enhanced adsorption and activation of N_2 reactants, thus significantly improving the photocatalytic nitrogen fixation performance.^[1-10]

Keywords: photocatalysis, defect, nitrogen fixation, layered double hydroxide

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SOLAR-ASSISTED CO₂ REDUCTION: FROM MECHANISTIC UNDERSTANDING TO DEVICE ENGINEERING

Jinlong Gong^{a,b,*}

^a*School of Chemical Engineering & Technology, Key Laboratory for Green Chemical Technology of Ministry of Education, Tianjin University; Collaborative Innovation Center for Chemical Science & Engineering; Tianjin, 300072, China.*

^b*Tianjin Normal University, Tianjin, 300387, China.*

**Corresponding author: jlgong@tju.edu.cn*

Abstract

Artificial photosynthesis is a key technology for achieving carbon neutrality and enabling a sustainable future. As a critical component of this process, solar-assisted (photo)electrochemical CO₂ reduction—the “dark reaction” of artificial photosynthesis—has garnered significant attention. Advancing this field requires both a deep mechanistic understanding and systematic engineering of the reaction systems. Through kinetic studies, we have identified the rate-determining steps for the formation of various products. By integrating theoretical calculations with in-situ spectroscopic techniques, we elucidate the relationship between active site structures and CO₂ conversion pathways. These mechanistic insights have informed the development of site-selective strategies for constructing highly active catalysts. Furthermore, using multiphysics simulations, we reveal how mass and charge transport processes influence the performance of membrane electrode assemblies, providing guidance for the scalable design of electrolyzers. Incorporating principles of energy coupling into system design has allowed us to establish matching criteria between solar energy input and electrolyzer operation. By optimizing temperature, flow dynamics, and concentration profiles, we demonstrate stable production of multi-carbon products under scalable conditions. Our work contributes to bridging the gap between fundamental research and practical implementation, advancing the development of efficient, solar-assisted CO₂ reduction systems.

Keywords: CO₂ reduction, photoelectrochemical, electrocatalysis, Cu catalysts

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DESIGN OF HETEROGENEOUS CATALYSTS FOR PRECISION CATALYSIS

Ye Wang*

^aState Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

**Corresponding author: wangye@xmu.edu.cn*

Abstract

The heterogeneous catalyst is typically composed of an active phase, a support and one or several promoters. Under the current pursuit of precision catalysis, developing new strategies for catalyst design has become imperative. Here, I present our catalyst-design strategies of dynamic control of confined single-atom catalysis for propane dehydrogenation and relay catalysis for syngas conversion to C₂ oxygenates.

Propane dehydrogenation (PDH) is one of the most attractive heterogeneous catalytic reactions, with a simple reaction mechanism mainly involving the C-H activation. However, fast catalyst deactivation due to the coke deposition, induced by the C-C cleavage and deep dehydrogenation, remains a significant challenge. Rhodium is the most active metal towards C-H activation, but Rh-based catalysts typically exhibit poor PDH performance. We successfully designed and constructed a highly efficient and ultrastable Rh single-atom catalyst by leveraging zeolite-confinement effect and the dynamic migration of indium species under reaction conditions.¹ No catalyst deactivation was observed for the conversion of pure propane at 550 °C over 6000 h.

Syngas (CO/H₂), a sustainable C1 feedstock derivable from either fossil resources or renewables, has attracted significant attention as a key platform. Despite remarkable advances in the conversion of syngas to lower olefins over the past decade, selective synthesis of a C₂ oxygenate from syngas, a reaction with complex mechanisms containing multiple intermediates and complex reaction networks, has been less successful. We demonstrate that relay catalysis is a promising methodology for designing catalyst to control such complex reactions.²⁻⁴ By designing and constructing a dual-site heterogeneous carbonylation catalyst that operates efficiently at a lower CO/CH₃OH ratio, we successfully overcame the conversion-selectivity trade-off in syngas conversion to C₂ oxygenates via relay catalysis. The selectivity of acetic acid or ethanol reached 90% at single-pass CO conversions of 30-40%.

Keywords: catalyst design, single-atom catalysis, relay catalysis, propane dehydrogenation, syngas conversions

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PRECISION CATALYSIS TOWARDS CARBON NEUTRALITY

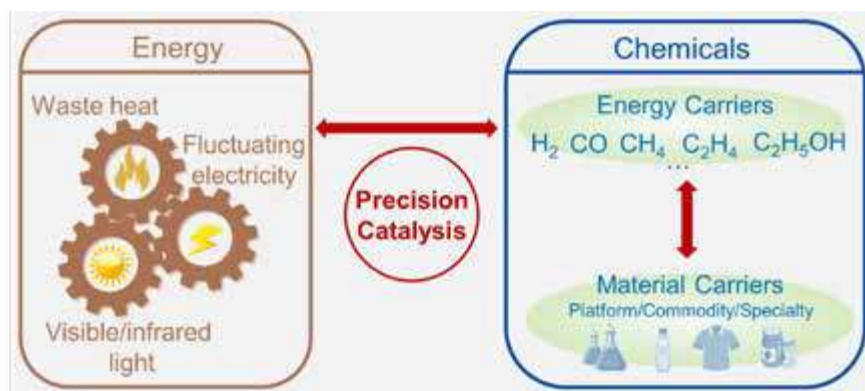
Gang Fu^{a,*}

^a*Collaborative Innovation Center of Chemistry for Energy Materials, State Key Laboratory for Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China*

^{*}*Corresponding author: gfu@xmu.edu.cn*

Abstract

Precision catalysis represents an emerging frontier vital to achieving global carbon neutrality goals. It encompasses targeted manipulation of catalytic systems to precisely control reaction outcomes, reduce environmental impact, and optimize renewable energy usage. Recent exemplary studies from our group highlight the successful application of precision catalysis across various scales, spanning from atomic-level active site optimization, surface dynamics and tailored reaction pathway. Targeting key reaction systems such as catalytic hydrogenation/dehydrogenation, we systematically reveal the electronic structure characteristics and dynamic evolution patterns of active sites on catalytic surfaces and interfaces through multi-scale simulation methods combining density functional theory, machine learning potential, and molecular dynamics. We specifically discuss several important catalytic systems: 1) the mechanism of alkyne semi-hydrogenation on alloy catalyst surfaces; 2) the influence of oxide surface/interface structures on CO₂ hydrogenation; 3) the formation mechanism of Rh-Inx single-atom alloy catalysts and their impact on the direct dehydrogenation of propane to propylene; 4) the regulation of B-based oxide coordination structures on C-H bond dissociation and O₂ activation in propane oxidative dehydrogenation. Furthermore, we outline the key challenges that lie ahead, as well as the critical research avenues required to propel the field forward. We focus on the cutting-edge advancements of theoretical chemistry methods in elucidating catalytic surface reaction mechanisms and rational catalyst design.



Keywords: DFT calculations, surface dynamics, strong metal-oxide interaction, alloy effect

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CARBON-BASED METAL-FREE ELECTROCATALYSTS FOR CLEAN ENERGY CONVERSION AND ENVIRONMENTAL REMEDICATION

Liming Dai

Australian Carbon Materials Centre

The ARC Centre of Excellence for Carbon Science and Innovation

University of New South Wales, Sydney, NSW 2052, Australia

Email: l.dai@unsw.edu.au; <https://www.carboncentre.org.au>

Abstract

Since our discovery of the first carbon-based metal-free electrocatalyst (C-MFEC, *i.e.*, N-doped carbon nanotubes) for oxygen reduction in fuel cells in 2009, the field of C-MFEC has grown enormously. C-MFECs, as alternatives to noble metal-based electrocatalysts, have been widely demonstrated for efficient oxygen reduction, oxygen evolution, hydrogen evolution, carbon dioxide reduction, nitrogen reduction, and many other electrocatalytic reactions. Recent worldwide research effort has shown great potential for applications of C-MFECs in fuel cells for clean energy conversion, metal-air batteries for energy storage, water splitting for hydrogen fuel generation, and other electrochemical processes for value-added chemical production to reduce or even eliminate greenhouse emissions. Further research and development of C-MFECs could revolutionize clean energy and environmental remediation technologies. In this talk, I will summarize some of our work on the development of C-MFECs for clean energy conversion and environmental remediation, along with an overview of recent advances, current challenges, and future perspectives in this exciting field.

THE INTERPLAY BETWEEN PLASMONICS AND ELECTROCHEMISTRY

Bin Ren, Xiang Wang, Yi-Fan Bao, Mengyuan Zhu, Teng-Xiang Huang

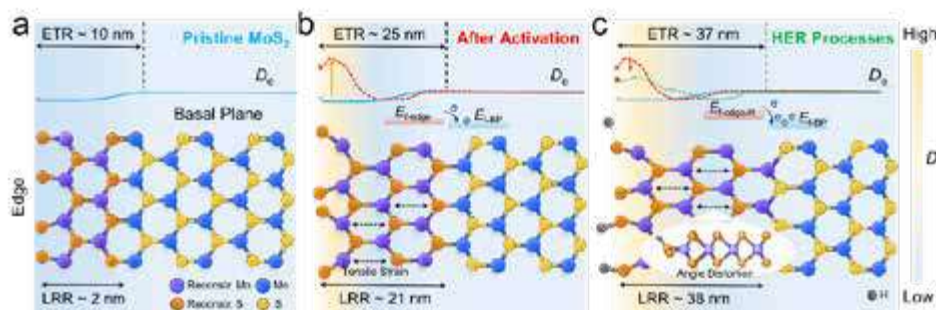
*State Key Laboratory of Physical Chemistry of Solid Surfaces, iChEM, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China
 Tan Kah Kee Innovation Laboratory, Xiamen 361005, China*

**Corresponding author: bren@xmu.edu.cn*

Abstract

Plasmonics is a rapidly evolving field, focusing on the interaction between light and metallic nanostructures of Au, Ag and Cu. The plasmonic excitation can create intense, localized EM fields near nanostructure surfaces due to the confinement of oscillating charges. This field enhancement, magnified at sharp tips or nanogaps amplifies optical signals such as Raman scattering, leading to some important techniques, such as surface-enhanced Raman spectroscopy (SERS) and tip-enhanced Raman spectroscopy (TERS). TERS, which can simultaneously provide topographic and chemical information, can provide very high spatial resolution down to sub-nanometer level in UHV condition and several nanometer under electrochemical condition. In this talk, we will bring you to the frontier of plasmonics and electrochemistry and how the effect as a result of the plasmonic excitation can be utilized to induce the electrochemical reaction and characterize the electrochemical processes. Special focus will be on the development of electrochemical TERS, from instrument construction to tip fabrication. We could achieve EC-TERS imaging with a spatial resolution of around 4 nm. EC-TERS was applied to probe the spatial distribution of plasmonically excited hot carriers, visualize the structural evolution of individual active sites of MoS₂ during hydrogen evolution reaction (HER), and detection of surface processes highly related to electrocatalytic processes, including CO adsorption and oxidation. We will point out the challenges and perspectives and how plasmonics can further propel the electrochemistry field.

Keywords: Electrochemistry, Raman, Carbon monoxide, active sites



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CARBON CAPTURE AND UTILIZATION FOR SUSTAINABLE VALUABLE PRODUCTS [CYCLIC CARBONATES, CARBON NEUTRAL FUEL - JET FUEL (SAF), METHANOL]

Mohd Rafie Bin Johan

Nanotechnology and Catalysis Research Center (NANOCAT), Universiti Malaya

**Corresponding author: mrafiej@um.edu.my*

Abstract

The conversion of CO₂ into high-value chemicals has become a significant research focus, attracting considerable attention from both academia and industry. Among the various CO₂ fixation processes, the catalytic one-pot synthesis of five-membered cyclic carbonates (CCs) through CO₂ incorporation with alkenes offers a greener, more sustainable alternative to traditional methods, such as phosgene-based processes and the cycloaddition of CO₂ with epoxides. The structural versatility of cyclic carbonates enables a wide range of applications, driving considerable efforts to identify efficient and practical catalysts for the oxidative carboxylation of alkenes with CO₂. This approach utilizes abundant, low-cost alkenes, and eliminates the need for separating and purifying intermediates, making it more economical and sustainable. However, despite significant advancements, the harsh reaction conditions—such as high temperatures, elevated pressures, and the use of toxic solvents and co-catalysts—remain obstacles to the industrial scalability of CO₂ valorization processes. In light of the shift towards a “sustainable society” and the promotion of “green chemistry,” there is a pressing need to develop efficient chemical processes for the catalytic valorization of CO₂ with alkenes under milder conditions. This work focuses on developing an efficient, environmentally friendly catalytic system for CO₂ valorization with alkenes, leading to the production of cyclic carbonates. The approach emphasizes the integration of a highly active catalyst, selective reaction conditions, and minimal solvent usage, achieving high yields of the desired products in a single reaction step. The reaction mechanism, scope, and various factors influencing the synthesis process are discussed, with an emphasis on scalability and potential industrial applications. This method presents a promising pathway for CO₂ utilization, contributing to the circular economy and reducing reliance on petroleum-based feedstocks for specialty chemicals.

Keywords: CO₂, Catalysis, Alkene, Oxidative carboxylation, Cyclic carbonate, Sustainable chemistry

MATERIALS FOR A SUSTAINABLE ENERGY FUTURE

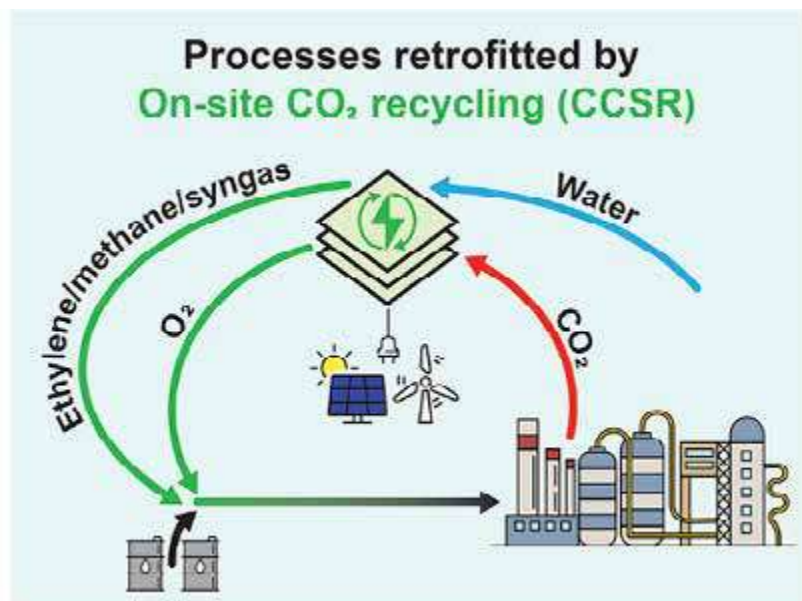
Professor Joel W. Ager^a

*^aAdjunct Professor in the Department of Materials Science & Engineering, University of California Berkeley and
Senior Scientist in the Materials and Chemical Sciences Divisions, Lawrence Berkeley National Laboratory*

Corresponding author: jwager@berkeley.edu

Abstract

If renewable power sources such as solar and wind could be used to produce chemical precursors and/or fuels, it would provide an alternative to mankind's accelerating use of fossil fuels and slow the rate of CO₂ emission into the atmosphere [1,2]. Photosynthesis provides a compelling example of light to chemical energy conversion and thus motivates work to make systems which achieve a similar function. Analogous to photovoltaics, driving the thermodynamically uphill redox reactions required for net solar to chemical energy conversion necessitates directional charge transport [3]. Additionally, to convert carbon dioxide to hydrocarbons, one must manage multi-electron transfer reactions (e.g. 12 in the case of ethylene and ethanol) [4]. Recent work in electrochemical CO₂ reduction (EC-CO₂R) will be discussed. Much of the current experimental research focuses on crafting active sites that will lower the overpotential and improve selectivity to either two-electron products (CO or formate/formic acid) or to specific C₂₊ products such as ethylene or ethanol. The experiments are often guided by DFT calculations of the binding energies and kinetic barriers between intermediate species involved in the individual proton-coupled electron transfer steps. This approach has yielded insights into the performance of nanostructured metal catalysts, single-atom catalysts, and immobilized molecular catalysts for EC-CO₂R [5]. However, recent work shows that the EC-CO₂R reaction environment is more diverse and dynamic than can be captured with this approach [6-8]. Moreover, the EC-CO₂R environment is highly dynamic, both at the atomic level driven by adsorbate-mediated surface reconstruction [9] and, in certain cases, at the macro-scale due to non-linear coupling of mass transfer and pressure [10]. Notably, many of these phenomena have analogies in heterogeneous thermal catalysis [11], and I will show that adapting classic surface science approaches for use in EC-CO₂R can yield key insights. Further, I will argue that the chemical reaction network of EC-CO₂R can have many of the functionalities found in biological networks such as inhibition/activation, cascades, and substrate channeling/pre-concentration. For this reason, adapting experimental and simulation methods from systems biology, in combination with chemical kinetics measurements, can yield mechanistic insights [12] and, prospectively, a predictive framework for EC-CO₂R. Despite this impressive progress in laboratory-scale CO₂ electrolysis, it is not yet directly competitive with existing, petroleum-based production methods. However, integration of CO₂ conversion into existing petrochemical plants is an attractive alternative. On-site CO₂ recycling (CCSR) in ethylene oxide production has a projected economic payback time as short as 1-2 years, depending on the availability of low-cost electricity and the applicable carbon taxes [13]. The CCSR approach is applicable to other large-scale chemical production processes including ammonia production. Wide-scale adoption of CCSR in chemical manufacturing has the potential to recycle between 4-10 Gt CO₂ annually by 2050, representing ca. 50% of this industry's carbon neutrality goal [14]. This work was supported by the National Research Foundation (NRF), Prime Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme through the eCO2EP project operated by Cambridge Centre for Advanced Research and Education in Singapore (CARES) and the Berkeley Education Alliance for Research in Singapore (BEARS) and by the AxClIS programme operated by BEARS.



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TOWARDS AI² ELECTROCHEMISTRY (AI² = AI × AB INITIO)

Jun Cheng^{a,b,c,*}

^aState Key Laboratory of Physical Chemistry of Solid Surfaces, iChEM,

^bCollege of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

^cLaboratory of AI for Electrochemistry (AI4EC), IKKEM, Xiamen, China

*Corresponding author: chengjun@xmu.edu.cn

Abstract

It is known that electrode materials undergo dynamic structural changes at in-situ/in-operando conditions. Yet, the majority of computational studies only consider the static structures of electrode materials. When the materials are submerged in liquid solution, dynamic solvation effects are often completely ignored, or treated with dielectric continuum models, often lacking validation. The situations are about to change. Thanks to the latest development of in-situ experimental techniques and state-of-the-art computational methods, dynamics of electrode materials has recently drawn more and more attentions in many research areas. In this talk, I will present our recent progress on modeling dynamic catalysis and electrochemistry using ab initio molecular dynamics (AIMD). The high computational cost of AIMD however limits its application to small model systems consisting of hundreds of atoms at timescale of tens of ps. While, the latest development of AI accelerated AIMD (AI²MD) significantly increases the size and timescale, showing great promise for in situ modeling of realistic electrochemical systems.

Keywords: electric double layer, dynamic catalysis, machine learning molecular dynamics, electrochemical interfaces

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METAL ORGANIC FRAMEWORKS FOR ENERGY APPLICATIONS: PERFECT MOFS, DEFECTIVE-, QUASI- AND POST-MOFS

John Wang

*Department of Materials Science and Engineering
National University of Singapore. Singapore 117574
NUS (Chongqing) Research Institute, China
Corresponding author: msewangj@nus.edu.sg

Abstract

Metal Organic Frameworks (MOFs) are undoubtedly among the most on-going and exciting materials for both energy conversion and energy storage applications. There is a huge number of them, including perfect MOFs, defective- and quasi-MOFs, and they exhibit extra high surface areas, tunable internal structures, and they can be both pre- and post-synthesis manipulated for almost whatever applications that are designed for them. Over the past decades, we have been exploring various new MOFs (also COFs) for applications in electrocatalysis, photocatalysis, various batteries (Lithium-sulfur, Zn aqueous and all solid-state batteries). In addition to MOFs and COFs themselves, we have also explored several classes of MOFs- tailored materials with better performance in energy conversion and energy storage applications, for example, including defective MOFs, quasi- and post-MOFs. In this talk, I will present several approaches that are aiming at better designing and fabricating new MOFs, their derivatives (e.g., defective and quasi-MOFs) for electrocatalysts, MOF-based electrolytes and cathode materials, together with key understandings that have been made so far. There are also several unsolved issues with them, especially in association with the formation, stability and service performance of these MOF-based/tailored materials, which will be highlighted in this presentation.

BATTERY INNOVATION EMPOWERED BY LITHIUM BOND AND ARTIFICIAL INTELLIGENCE

Xiang Chen, Chen-Zi Zhao, Xi-Yao Li, Yu-Chen Gao, Xue-Yan Huang, Qiang Zhang*

Beijing Key Laboratory of Complex Solid State Batteries, State Key Laboratory of Chemical Engineering and Low-Carbon Technology, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

**Corresponding author: zhang-qiang@mails.tsinghua.edu.cn*

Abstract

Lithium bonds, analogous to hydrogen bonds, exhibit unique properties due to lithium's weak metallic nature, offering exciting potential for lithium battery applications. This talk will delve into the concept of lithium bonds, exploring their underlying chemistry and how they can be harnessed to design new battery material combining with emerging artificial intelligence and further improve battery performances. Specifically, solid electrolytes combined with high-voltage Li-rich Mn-based cathodes and anode-free cell designs hold significant promise for high-energy-density and high-safety systems. However, challenges such as interfacial oxygen escape and unstable anode morphology continue to hinder their widespread applications. To address these issues, we have developed a fluoropolyether-based solid polymer electrolyte featuring a novel anion-rich solvation structure, which stabilizes the interface and enhances cycling stability. The resulting pouch cell demonstrates an ultra-high energy density (>600 Wh/kg) and excellent safety under a nail penetration at a full charge condition, advancing solid-state battery technology and paving the way for safer, higher-energy systems.

Keywords: lithium bonds, artificial intelligence, high-energy-density rechargeable batteries, lithium metal anode, solid electrolyte interphase

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***IN SITU/OPERANDO* RAMAN SPECTROSCOPY STUDIES OF HYDROGEN FUEL CELL REACTIONS**

Jin-Chao Dong^{a*}

^a*College of Energy, Xiamen University, Xiamen 361005, China.*

^{*}*Corresponding author: jcdong@xmu.edu.cn*

Abstract

Hydrogen fuel cell technology, known for its cleanliness and high energy efficiency, has garnered significant attention. The electrocatalytic reactions occurring at the catalyst interface of hydrogen fuel cells involve critical information regarding complex charge transfer, species evolution, and energy transfer. *In situ* investigations of these electrocatalytic processes in fuel cells will provide the most direct insights for elucidating structure-activity relationships, deepening our understanding of reaction mechanisms, and guiding the design of high-efficiency catalytic materials. As a fingerprint spectroscopic technique with exceptional surface sensitivity, surface-enhanced Raman spectroscopy (SERS) offers direct spectral evidence for trace intermediate species and adsorbed molecules at catalyst surfaces/interfaces, free from aqueous interference, making it particularly suitable for studying electrocatalytic mechanisms at solid-liquid interfaces. Leveraging surface plasmon-enhanced strategies, we have developed and employed a series of highly sensitive *in situ/operando* electrochemical Raman spectroscopy techniques. These methodologies were systematically applied to investigate critical electrocatalytic processes in hydrogen fuel cells across various catalytic interfaces, including single-crystal catalysts, core-shell catalysts, and practical catalyst systems. Key reactions such as the oxygen reduction reaction (ORR), hydrogen oxidation reaction (HOR), and anti-poisoning reactions were examined, successfully capturing direct spectroscopic evidence of crucial reaction intermediates including OOH*, OH*, and H*.¹⁻⁵ Through combined theoretical calculations and analysis of these intermediate species and surface-adsorbed moieties revealed by Raman spectroscopy, we established correlations between structural characteristics and catalytic performance. This integrated approach not only provides fundamental insights into the nature of electrocatalytic reactions but also offers practical guidance for optimizing the design and fabrication of advanced hydrogen fuel cell catalysts.

Keywords: Hydrogen fuel cells, electrocatalytic reactions, SERS, reaction intermediates, structure-activity relationship

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CATALYTIC DEPOLYMERIZATION OF POLYETHYLENE AND POLYSTYRENE

Jason Y. C. Lim^{a*}, Tristan T. Y. Tan^a, Albert Ong^a

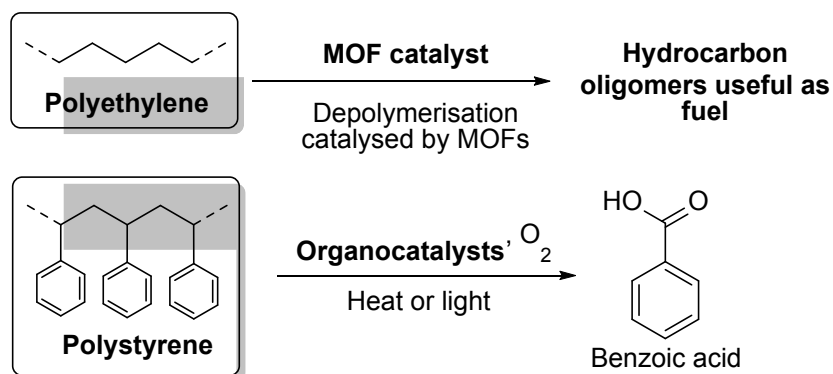
^a*Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR),
2 Fusionopolis Way, Innovis #08-03, Singapore 138634, Republic of Singapore*

**Corresponding author: jason_lim@imre.a-star.edu.sg*

Abstract

Plastics containing saturated C-C backbones make up close to 60% of the 380 million tonnes produced annually, and include some of the most environmentally-recalcitrant polymers such as polyethylenes (PEs) and polystyrene (PS). The lack of cleavable bonds in their polymer backbones make them highly challenging to break down, necessitating development of innovative catalysts for their depolymerization into industrially-relevant chemicals.¹ Herein, we discuss some of the emerging strategies for PE and PS depolymerization recently developed by our team. These include the exploitation of highly-designable metal organic frameworks (MOFs) as a new class of catalysts for PE depolymerization into hydrocarbons,² with complementary product selectivity to zeolites. Additionally, the use of organocatalysts to upcycle PS into benzoic acid under mild thermal and photocatalytic conditions will be explored. These findings set the scene for exploiting waste plastics as viable feedstock for production of chemicals and functional materials for a future circular economy.³

Keywords: polyolefins, chemical recycling, plastic upcycling, pyrolysis, fuels



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CATALYTIC TRANSFORMATION OF WATER POLLUTANTS VIA NONRADICAL OXIDATION

Xiaoguang Duan^{a,*}

^a School of Chemical Engineering, The University of Adelaide, Adelaide, Austral

*Corresponding author: xiaoguang.duan@adelaide.edu.au

Abstract

The critical environmental issues urge advanced and green technologies for the purification of contaminated water systems due to the existence of diverse hazardous organic substances produced from human activities. In addition to classic physical separation (e.g., flocculation and membranes) and bio-processes (aerobic/anaerobic digestion), advanced oxidation processes (AOP) are highly efficient to purify organic pollutants and pathogens. In this presentation, we will introduce our recent findings of catalytic conversion of organic pollutants into polymers to realise organic pollutant migration from wastewater onto the solid phase. We find that nanocarbons and metal oxides can activate persulfates (peroxymonosulfate-PMS and peroxydisulfate-PDS) to coordinate a nonradical electron-transfer pathway (ETP). [1,2] The ETP oxidation regime featured a mild oxidation potential and high selectivity toward electron-rich micropollutants in complicated water matrixes via electron transfer and hydrogen abstraction reactions. More intriguingly, phenolics and similar substituted compounds will be selectively converted into their corresponding dimers, trimers, and polymeric compounds. [3,4] Such a process will remarkably reduce the dosage of persulfate to minimise the chemical input in AOP and realise the upgrading of organic pollutants to value-added polymers. Via spatially separating PMS activation sites on high entropy alloys (HEAs) and organic polymerization on carbon substrate (NG), the HEA@NG composites enabled sustained pollutant removal with high electron utilization efficiency. The new remediation system will help mitigate carbon emissions in water treatment processes to realise pollutant to value-added product transformation.

Keywords: Micropollutants, electron transfer, advanced oxidation, nonradical, polymerization.

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SELF-SUPPORTED BIFUNCTIONAL $\text{Zn}_x\text{Co}_y\text{S}$ CATALYST MATERIALS FOR ALKALINE WATER SPLITTING

Nor Atikah Abu Bakar, Kee Shyuan Loh*, Wai Yin Wong, Kean Long Lim,
Rozaan Mohamad Yunus

Fuel Cell Institute, Universiti Kebangsaan Malaysia, 43000, Bandar Baru Bangi, Selangor, Malaysia

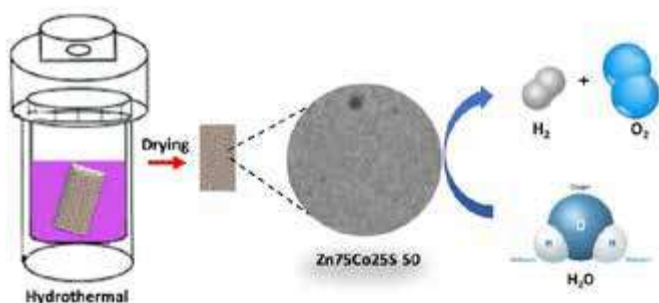
*Corresponding author: ksloh@ukm.edu.my

Abstract

Developing highly efficient catalysts using simple methods is crucial for accelerating the slow reaction kinetics of the alkaline hydrogen evolution (HER) and oxygen evolution (OER) processes, ensuring cost-effective hydrogen and oxygen production. In this study, a two-step hydrothermal method was successfully employed to synthesize CoS and $\text{Zn}_x\text{Co}_y\text{S}$ on a Ni foam substrate. The parameters studied in this research were the synthesis temperature and the Zn:Co ratio. The results indicated that the addition of Zn to pristine CoS affected morphology due to the presence of Zn ions, promoting the transformation of mossy-like CoS into corals-like nanorod-shaped $\text{Zn}_x\text{Co}_y\text{S}$. During hydrothermal synthesis, ZnCoS was directly deposited onto the surface of Ni foam, creating a roughened texture with increased troughs between the grains, thereby enhancing mass transport during electrochemical reactions. The synthesized $\text{Zn}_{75}\text{Co}_{25}\text{S}/\text{NF}$ at 50 °C exhibited improved HER and OER performance, with overpotential of 178 mV at $-10 \text{ mA}/\text{cm}^2$ and 364 mV at $10 \text{ mA}/\text{cm}^2$, respectively. The catalyst also demonstrated enhanced HER and OER kinetics, with Tafel slope of 94.8 mV/dec and 74.4 mV/dec, respectively, compared to the pristine catalyst. This study presents an intuitive synthetic approach for developing effective non-noble metal catalysts for alkaline hydrogen evolution reaction and overall water splitting.

Keywords: Water electrolyser, catalysts, HER, OER, anion exchange membrane water electrolyser

Graphic / Image



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DEVELOPMENT OF SUSTAINABLE CHEMICAL TRANSFORMATIONS VIA RATIONALLY DESIGNED HETEROJUNCTION PHOTOCATALYSTS

Önder Metin

Department of Chemistry, College of Sciences, Koç University, Istanbul, Türkiye

Koç University Hydrogen Technologies Center (KUHyTech)

**Corresponding author: ometin@ku.edu.tr*

Abstract

Among basic sciences, chemistry plays a key role in achieving sustainability, as the production of most goods requires one or more chemical processes. One of the most promising strategies in Green Chemistry is the use of photocatalysts that can absorb a significant portion of the sunlight spectrum to drive chemical reactions consistent with its twelve principles [1]. Semiconductor materials have been investigated as photocatalysts for a variety of chemical transformations hitherto. However, the use of pristine semiconductors is often limited by challenges such as improper band alignment and problems with electron-hole recombination in photocatalytic applications. To overcome these challenges, several strategies have been developed, including converting semiconductors from 3D bulk forms to 0D, 1D, and 2D structures and designing heterojunctions to facilitate efficient charge separation. As a result, two-dimensional (2D) transition metal-based semiconductors such as metal dichalcogenides and metal-free materials (graphitic carbon nitride (gCN) and black phosphorus (BP)) have emerged as viable photocatalysts for various chemical reactions [2]. However, like most semiconductor photocatalysts, these materials face common limitations such as absorbing only a small portion of the solar spectrum or suffering from photogenerated electron-hole (e^-h^+) recombination. An efficient e^-h^+ separation and significant visible-light absorption are essential to create an effective photocatalyst for any chemical transformation, and numerous techniques have been developed to achieve this goal [3]. Owing to the large surface and interfacial area of heterojunctions, photogenerated e^-h^+ pairs can be rapidly transferred across the interface [4]. In recent years, we have developed heterojunction photocatalysts based on gCN and/or BP for various chemical reactions. In this talk, I will discuss our latest research activities on the rational design of gCN and/or BP based heterojunction photocatalysts for hydrogen production from water and other chemical hydrogen storage materials, photoredox C-H functionalization, and hydrogen peroxide production.

Keywords: Green Chemistry, Photocatalysis, Heterojunction Photocatalyst, Hydrogen Production, Photoredox C-H Functionalization.

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MECHANISM ON ARTIFICIAL PHOTOSYNTHESIS OF H_2O_2 : A C_3N_4 SURFACE STUDY

Pengxin Liu^{a,*}

^a*School of Physical Science and Technology, ShanghaiTech University, Shanghai, P. R. China*

^{*}*Corresponding author: liupx@shanghaitech.edu.cn*

Abstract

Photocatalytic generation of H_2O_2 is a promising, green and sustainable process that utilizes solar energy to convert water (H_2O) and O_2 , replacing the industrial process through anthraquinone oxidation (AO). Previous optimization of the photocatalysts mainly focused on three aspects, namely increasing the light adsorption, enhancing the charge separation, and boosting surface reactions. However, the trials based on doping and surface modification of photocatalysts may change the reaction pathways, making the efforts aimless. The surface chemistry of nanocatalysts should be considered [1-5]. In this talk, some findings on the reaction mechanism of photocatalytic generation of H_2O_2 will be discussed, including the influence of sacrifice agents, the surface H-transfer, and isotopic effects.

Keywords: Surface coordination chemistry; 2D material; C_3N_4 ;

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FUNDAMENTAL PERSPECTIVES GUIDING THE RATIONAL DESIGN OF TM-N-C-BASED OXYGEN REDUCTION REACTION CATALYSTS FOR PEM FUEL CELLS

Wai Yin Wong

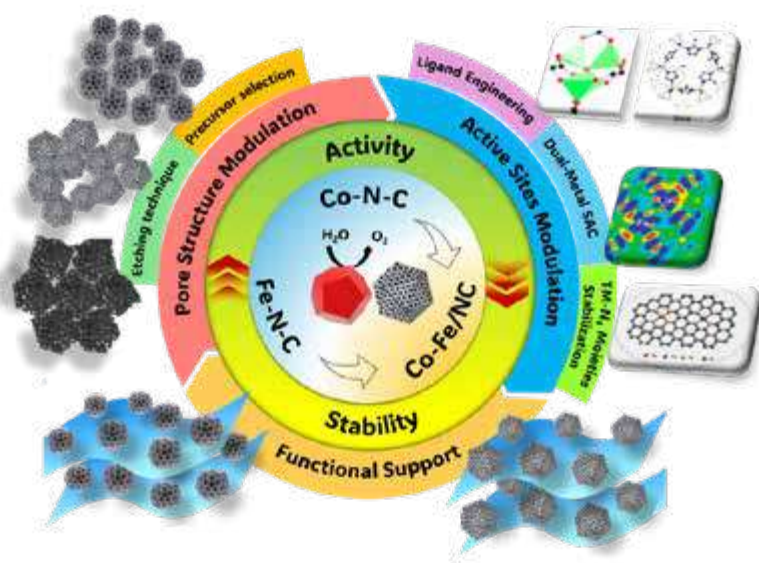
Fuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.

Corresponding author: waiyin.wong@ukm.edu.my

Abstract

The urgent need for sustainable energy technologies has intensified the search for efficient, platinum-free oxygen reduction reaction (ORR) catalysts. Metal-organic framework (MOF)-derived transition metal-nitrogen-carbon (TM-N-C) materials have emerged as leading candidates due to their tunable atomic architectures, high surface areas, and potential for single-atom active sites. However, widespread adoption of TM-N-C catalysts in proton exchange membrane fuel cells (PEMFCs) remains hindered by challenges including intrinsic activity limitations, durability issues, and incomplete mechanistic understanding under operational conditions. This lecture will present fundamental perspectives on the rational design of MOF-derived TM-N-C systems, addressing: (1) electronic structure modulation of M-N_x sites to enhance intrinsic activity; (2) pore engineering strategies to optimize mass transport and accessibility; and (3) hybrid architectures with supportive materials (e.g., conductive carbons or metal oxides) to improve stability. By correlating synthesis approaches, including precursor selection, pyrolysis control, and post-treatment modifications - with electrochemical performance, this lecture will highlight how structure-property relationships serve as critical factors for advancing these catalysts.

Keywords: Fuel Cells, oxygen reduction reaction, TM-N-C; rational design; active sites



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CARBON-NEUTRAL PRODUCTION OF CARBON NANOTUBES FROM PLASTIC AND BIOMASS WASTE VIA CATALYST DESIGN

Wen-Da Oh^{a,*}, Xiu-Xian Lim^a

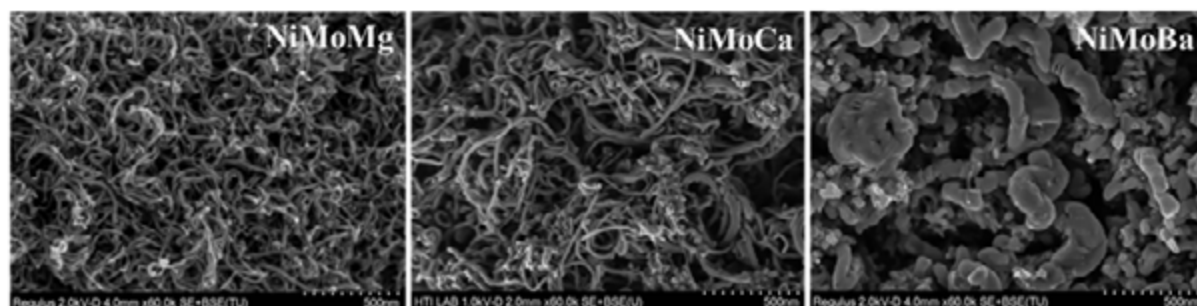
^a*School of Chemical Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia*

**Corresponding author: ohwenda@usm.my*

Abstract

The increasing accumulation of plastic and biomass waste, coupled with a lack of proper management strategies, has resulted in significant environmental challenges. An innovative waste-to-resources strategy can be adopted as an effective approach to manage these wastes while generating economic benefits. Plastic and biomass waste can be transformed into carbon nanotubes (CNTs) via catalytic pyrolysis processes. The catalyst design is a crucial determinant of process efficiency and CNTs characteristics. In this study, Ni-based catalysts consisting of NiMoCa-X (X = 0, 7, 15, 32 wt.% of Ca) were designed and used to produce CNTs from polypropylene and lignocellulosic biomass via one-pot catalytic processes. Notably, NiMoCa-15 exhibited the highest carbon yield and CNTs quality attributed to its smaller NiO crystallite size and enhanced surface basicity¹. Excessive Ca loading (NiMoCa-32) resulted in aggressive coke gasification and shorter CNTs. The incorporation of Ca plays a vital role in tuning catalytic performance through the formation of CaMoO₄ and CaCO₃ phases, enhancing the carbon diffusion into Ni active sites. Specifically, CaMoO₄ facilitates surface coke oxidation and CaCO₃ promotes aromatization reactions, yielding high-quality CNTs. Comparative studies with NiMoMg-15 and NiMoBa-15 further highlighted the superior carbon recovery of NiMoCa-15, which creates a low CO₂/CH₄ environment via CO₂ methanation, while NiMoMg-15 produced thinner CNTs, whereas NiMo-Ba promoted the formation of irregular carbon flakes². Additionally, polypropylene produced high-quality CNTs with 5-6 wt.% carbon yield, whereas blending plastics with lignocellulosic biomass can increase the carbon yield up to 11 wt.% at the expense of the CNT quality. These findings provide critical insights into catalyst engineering for efficient waste-to-CNTs conversion, supporting the advancement of carbon-neutral nanomaterial production within a circular economy framework.

Keywords: Ni-based catalyst; Carbon Nanotubes; One-pot pyrolysis; Catalyst design; Waste-to-Resources



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ENGINEERING THE ELECTRONIC STRUCTURE OF RU-BASED NANOCATALYSTS FOR EFFICIENT PHOTO-THERMAL CATALYTIC CO₂ CONVERSION

Fenglong Wang*¹

¹*School of Materials Science and Engineering, Shandong University, Jinan, China*

**Corresponding author: fenglong.wang@sdu.edu.cn*

Abstract

Photo-thermal catalytic hydrogenation of CO₂ into value-added chemicals under mild conditions has garnered global interest, yet achieving high conversion efficiency and selectivity remains challenging. To address these obstacles, we fabricated series of Ru-based catalysts. Firstly, Ru nanoparticles were dispersed on a narrow bandgap MnCo₂O₄ semiconductor, forming a composite catalyst. Under visible light irradiation, electron transfer from MnCo₂O₄ to Ru, which enhances charge separation and therefore promoted reactant adsorption and activation. Additionally, the strong light absorption and photothermal conversion capacity of create MnCo₂O₄ a local electromagnetic field, raising the active site temperature and boosting reaction rates. Secondly, in order to reduce the cost of Ru-based catalysts, we synthesized monodispersed Ru_xCo_{1-x} alloy nanoparticles via a one-step hydrothermal method and loaded onto TiO₂ nanosheets, and the composites show efficient CO₂ transformation due to tunable electronic structures and optimized carrier separation. Lastly, single-atom Ru catalysts with Ru-F₄ and Ru-O₄ configurations demonstrate enhanced performance in CO₂ hydrogenation to methane, with Ru-F₄ outperforming Ru-O₄. These findings offer new strategies for designing efficient photothermal catalysts for CO₂ methanation with optimized noble metal utilization.

Keywords: photothermal catalysis, heterogeneous catalysis, CO₂ conversion, solar fuels, hydrogenation

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ACTIVATION OF SMALL MOLECULES (CO₂, N₂) WITH CATALYSIS, HEAT, AND LIGHT

Jennifer Strunk^{a,b,*}

^aTechnical University of Munich, School of Natural Sciences, Germany.

^bLeibniz Institute for Catalysis at the University of Rostock, Germany.

*Corresponding author: Jennifer.strunk@tum.de

Abstract

In decades of work, it has been attempted to reduce CO₂ to valuable products by photocatalysis at room temperature. However, yield improvements were limited, with industrial application not yet realized. Thermal heterogeneous catalysis for CO₂ reduction, on the other hand, is performed in industrial processes such as methanol synthesis and the reverse water gas shift reaction (RWGS). Here, however, hydrogen is needed, and the reactions are run at elevated pressure, which leads to high CO₂ emissions rather than carbon emission reduction.

We combine the benefits of both approaches, by a primary direct action of the photogenerated charge carriers like in photocatalysis, but at elevated temperatures and mildly elevated pressures. First, it will be shown that reliable and reproducible reaction conditions in photocatalytic CO₂ reduction are difficult to achieve [1]. Then it will be demonstrated that similar (nano)catalysts can be used as in thermal catalysis, provided that the materials contain at least one suitable light-absorbing compound [2]. Detailed studies with Cu/ZnO/Al₂O₃ catalysts – known from industrial methanol synthesis and (R)WGS – demonstrate that the exact choice of the reaction conditions (p, T, light source) strongly influences product distribution, whereby either the formation of CO or methanol can be selectively enhanced [3].

In the last part of the talk, the same concept is adopted for oxidative dinitrogen activation with the aim to produce nitric acid “from thin air”. Active sites known from classical catalysis for nitrogen splitting and NO_x reactions are anchored onto TiO₂, and the formation of surface nitrates from N₂ and O₂ is demonstrated by IR spectroscopy. Gaseous water and native surface species (e.g. carbonates) are shown to influence the performance [4].

Keywords: photocatalysis, CO₂ reduction, dinitrogen activation, sustainable production, active sites

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ENGINEERED CATALYSTS FOR GREEN HYDROGEN PEROXIDE PRODUCTION

Xiangkang Zeng^{a*}

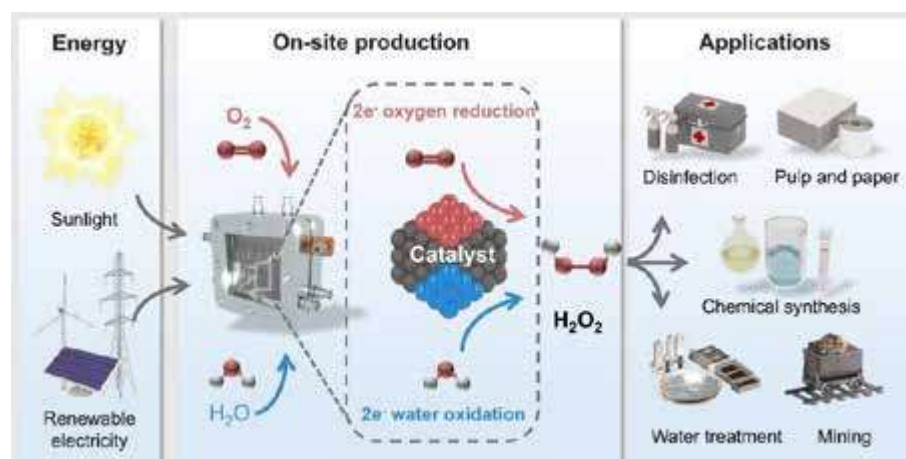
^a UQ DOW Centre, School of Chemical Engineering, The University of Queensland, St. Lucia, Brisbane, QLD, 4072 Australia

*Corresponding author: x.zeng@uq.edu.au

Abstract

Photocatalysis and electrocatalysis hydrogen peroxide (H_2O_2) production has gained broad research attention since it is a potentially viable route for “green” on-site H_2O_2 manufacturing from just water and oxygen using renewable solar energy^{1,2}. In the past decade, stunning progress has been made. However, efficient catalysts are still in need to push the current boundaries of H_2O_2 production in terms of generation rate and product concentration³. Besides, a fit-for-purpose application is needed to demonstrate its practical use. In this presentation, we will talk about our recent works on the rational design of photocatalysts and electrocatalysts for improved H_2O_2 production⁴⁻⁶. Additionally, the application for disinfection of bacteria in water will also be covered. It is expected to provide insights on designing catalysts with judicious structures and function for environmental applications via green catalysis process.

Keywords: hydrogen peroxide, electrocatalysis, photocatalysis



Schematic diagram of the on-site H_2O_2 synthesis by photocatalytic and electrocatalytic processes and its applications¹

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GREEN ELECTROCHEMICAL ENGINEERING FOR A SUSTAINABLE FUTURE

Fengwang Li^{a,*}

^a*The University of Sydney.*

**Corresponding author: fengwang.li@sydney.edu.au*

Abstract

Electrochemical engineering is playing an increasingly vital role in addressing global sustainability challenges, offering innovative solutions for cleaner energy and chemical production. In this seminar, I will share my research journey in leveraging the power of electrochemistry to contribute to a more sustainable future. My presentation will focus on two key areas. Firstly, I will discuss my work on circular carbon strategies, detailing the development of efficient electrocatalytic systems for capturing and converting CO₂ into valuable chemicals and fuels. This includes exploring new catalyst designs, reaction mechanism understanding, and reactor architectures aimed at closing the carbon loop. Secondly, I will discuss my research on green ammonia, covering both sustainable production routes using electrochemical methods powered by renewable energy, and innovative approaches to electrochemical ammonia cracking for on-demand hydrogen generation. I will highlight the key findings, impactful outcomes, and future directions of these projects, showcasing how electrochemical innovations can contribute to a greener and more sustainable energy and chemical landscape.

Keywords: electrocatalysis, CO₂ reduction, ammonia, hydrogen

COUPLED PHOTOELECTROCHEMICAL H₂ PRODUCTION AND SYNTHESIS OF VALUABLE CHEMICALS

Fatwa F. Abdi^{a,*}

^a*School of Energy and Environment, City University of Hong Kong.*

^{*}*Corresponding author: ffabdi@cityu.edu.hk*

Abstract

Green H₂ has been widely proposed as a key solution for decarbonizing our fossil fuel-dependent society. One promising method for producing it is solar water splitting via photoelectrochemical (PEC) devices. While solar-to-hydrogen (STH) efficiencies of up to 30% have been achieved, these high-performance systems rely on expensive, non-scalable photoelectrodes,¹ making the resulting hydrogen cost non-competitive. To address this challenge, low-cost, high-efficiency alternatives, such as earth-abundant complex metal oxides, are explored. Our recent works focused on developing bismuth vanadate and tin tungstate as promising photoelectrode materials will be discussed.²⁻⁶ Another strategy to improve economic viability is integrating valuable chemical production within the PEC system. For instance, we recently demonstrated a device that couples homogeneous hydrogenation with PEC-generated hydrogen. Using the conversion of itaconic acid (IA) to methyl succinic acid (MSA) as a proof of concept, our bismuth vanadate-based PEC device achieved a solar-driven H₂-to-MSA conversion efficiency of ~50%.⁷ Although still at the laboratory scale, life-cycle net energy assessments and technoeconomic analyses confirm the approach's strong potential.^{8,9} Finally, we will discuss further optimization opportunities, including high-pressure operation for broader hydrogenation applications and alternative oxidation reactions.¹⁰⁻¹²

Keywords: Photoelectrochemistry, green hydrogen, green chemical synthesis, hydrogenation, complex metal oxide

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OPTIMIZING $\text{CuS}_x/\text{CoS}_x$ ELECTROCATALYSTS VIA SULFIDATION FOR SUSTAINABLE GREEN HYDROGEN PRODUCTION FROM SEAWATER

M. Mottakin^{1,2}, Mohd Sukor Su'ait^{1*}

¹*Solar Energy Research Institute (SERI), Universiti Kebangsaan Malaysia (UKM), Bangi 43600, Selangor, Malaysia*

²*Gopalganj Science and Technology University (GSTU), Gopalganj-8105, Bangladesh*

**Corresponding Author: mohdsukor@ukm.edu.my*

Abstract

This study presents the development of a bifunctional electrocatalyst comprising sandwich design of $\text{CuS}_x/\text{CoS}_x$, sequentially deposited on nickel foam (NF) via an electrodeposition–sulfidation method. In this sandwich design configuration, the bottom CuS_x layer enhances charge transport, while the top CoS_x layer functions as the primary catalytic surface. Here, the role of sulfur incorporation in optimizing this structure is systematically investigated. Field emission scanning electron microscopy (FESEM) reveals that optimized sulfidation results in a rice-germination-like morphology, maximizing exposure of active sites. The synergistic effect between CuS_x and CoS_x leads to excellent electrocatalytic performance. Sulfidation with 0.1 M sodium sulfide yields overpotentials at 100 mA/cm^2 (η_{100}) of 387 mV for the oxygen evolution reaction (OER) and 259 mV for the hydrogen evolution reaction (HER). Tafel slopes of 20 mV/dec for OER and 162 mV/dec for HER further indicate favorable OER kinetics. The composite electrode exhibits strong durability, maintaining performance over 48 hours of OER and 200 hours of HER in alkaline seawater. This work offers valuable insights into layered catalyst engineering for efficient and sustainable green hydrogen production from seawater.

Keywords: Electrocatalysts, Sulfidation, Oxygen evolution reaction (OER), Hydrogen evolution reaction (HER), Seawater, Green Hydrogen

PLASMON-MEDIATED CHEMICAL PROCESSES

Chao Zhan^{a,*}, Zhong-Qun Tian^a,

^a State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering,
Collaborative Innovation Center of Chemistry for Energy Materials (iChEM), Xiamen University,
Xiamen 361005, China

*Corresponding author: zc@xmu.edu.cn

Abstract

Plasmonic devices based on surface plasmons excitation—collective oscillation of conduction-band electrons in nanostructures—can overcome the optical diffraction limit to provide pathways to detect, modulate and generate light in nano-scale, deriving numerous nanophotonics technologies. Such. Recently, there has been a new field based on the surface plasmons (SPs) to harvest or redistribute the incident light for an efficient utilization of solar energy and photochemistry. [1]

These years, we tried to investigate the photoelectrochemical response of the plasmonic nanostructures and discovered that the photocurrent behaviors of the metal nanostructures with SPs are quite different from that of semiconductors because of the lack of band gap. The plasmonic photocurrents can be enhanced at both negative and positive potentials, thereby promoting either reduction reactions by excited electrons or oxidation reactions by excited holes, contrasting with semiconductor-based photoelectrochemistry. [2] And the plasmonic photocurrent consists of two components: a rapid response current and a slow response current, corresponding to the photoelectronic and photothermal effects. Thus, photoelectrochemical method has become a widely used method to disentangle the photothermal and photoelectronic effects of plasmonic metal nanostructure. Recently, combining the photoelectrochemical method with the dark field scattering spectroscopy, we tried to reveal the charge and energy flow at metal-molecule interface, especially detangling the direct electron transfer from indirect electron transfer. [3]

Then, we used the plasmonic nanostructure as a strategy to regulate the electrochemical process for energy and/or chemical conversion, including electrochemical ethanol, formic acid oxidation and CO₂ reduction, during which the electrical and optical energy coupled at the electrochemical interface and could effectively regulate and improve the chemical reaction path selectively. [4] These recent experimental and theoretical approaches will be discussed in details.

Keywords: Surface plasmons, photoelectrochemistry, metal-molecular interface

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IMMOBILIZING IONOMERS BY HYDROGEN BOND NETWORKS FOR HIGHLY STABLE WATER ELECTROLYSIS AT 3.0 ACM²

Hua Bing Tao^{a,b*}, Han Liu^{a,b}, Nanfeng Zheng^{a,b}

^aState Key Laboratory for Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, and College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

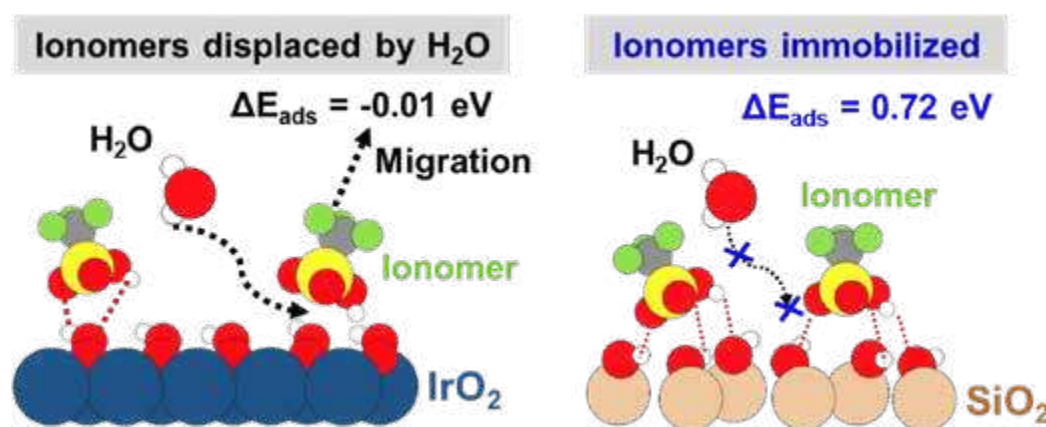
^bInnovation Laboratory for Sciences and Technologies of Energy Materials of Fujian Province (IKKEM), Xiamen 361005, China

Corresponding author: hbtao@xmu.edu.cn (H. B. T.)

Abstract

Increasing the current density can effectively reduce the high cost of proton exchange membrane water electrolyzers (PEMWEs). However, this approach is constrained by rapid performance degradation due to the increased mass transport resistance. We identified a critical degradation mechanism in which ionomer migration obstructs mass transport channels in the anode catalyst layer (ACL)¹⁻⁴. This work further demonstrated that ionomer migration is caused by weak adsorption of ionomer on IrO₂ surface, which can be easily displaced by water molecule due to the low adsorption energy difference. To immobilize ionomers, we proposed to introduce new sites to specially construct strong hydrogen bond with sulfonate groups from ionomer. Ionomers were successfully immobilized by highly acidic hydroxyl groups. Consequently, the optimized ACL showed a fourfold reduction in decay rate over 2500 hours of operation at 3.0 A/cm². Benefit from the significantly improved stability of catalyst ink, the strong hydrogen bond ACL was demonstrated to be easily scaled up to 600 cm² electrode and 35 kW stack, showing an excellent performance that meets the 2026 DOE targets.

Keywords: PEM water electrolysis, anode catalyst layer, durability, high current density, ionomer migration, hydrogen bond.



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ELECTROSYNTHESIS OF FUELS AND CHEMICALS: FROM ELECTROLYZERS TO BATTEROLYZERS

Hanfeng Liang*

*State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering,
Xiamen University, Xiamen 361005, China*

**Corresponding author: hfliang@xmu.edu.cn*

Abstract

Electrosynthesis has emerged as a highly promising method for synthesizing high-value-added fuels and chemicals (e.g., hydrogen, ammonia, carbohydrate, and organic molecules), which are traditionally produced through methods that often involve intensive energy consumption and greenhouse emissions. Despite its potential, the electrosynthesis of fuels and chemicals currently suffers from large overpotential due to the sluggish reaction kinetics, resulting in high energy input.

In this talk, we will demonstrate how the efficiency of the electrosynthesis can be improved through catalyst design and reaction pathway regulation. Additionally, we will introduce a novel type of electrochemical cells, the batterolyzers, which can produce valuable chemicals such as H₂ and NH₃ like an electrolyzer while simultaneously generating electricity like a battery. We have developed three types of batterolyzers: acid-base asymmetric cells, metal anode cells, and effluent-based cells, each offering unique benefits for high-value-added chemical production from low-quality water and generating electricity.

Keywords: batterolyzer, catalyst, chemical synthesis, electricity generation

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POLYANILINE INTEGRATED HYDROXYL FUNCTIONALIZED g-C₃N₄ WITH SYNERGISTIC INTERFACIAL DESIGN FOR ENHANCED PHOTOCATALYTIC HYDROGEN PEROXIDE PRODUCTION

Nur Shamimie Nadzwin Hasnan^{a,b}, Mohamad Azuwa Mohamed^{a,c*}, Wan Nor Roslam Wan Isahak^d,
Mohammad B. Kassim^{a,c}, Pragati A. Shinde^b, Renzhi Ma^b, Yu Yamashita^b, Katsuhiko Ariga^{b,e},
Lok Kumar Shrestha^{b,f}

^aDepartment of Chemicals Science, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.

^bResearch Center for Materials Nanoarchitectonics (MANA), National Institute for Material Science (NIMS), 1-1 Namiki, Tsukuba, 305-0040 Ibaraki, Japan.

^cFuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Malaysia.

^dDepartment of Chemical Process and Process Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.

^eDepartment of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa 277-8561, Chiba, Japan.

^fDepartment of Materials Science, Institute of Pure and Applied Sciences, University of Tsukuba, 1-1-1, Tennodai, Tsukuba 305-8573, Ibaraki, Japan.

*Corresponding author: mazuwa@ukm.edu.my

Abstract

Graphitic carbon nitride (g-C₃N₄) has emerged as an innovative non-metal-based photocatalyst with a tunable band gap and active under visible light. However, its practicability is hindered by inherent limitations such as insufficient light absorption, low surface area, inefficient charge transportation and rapid recombination of photogenerated electron-hole pairs. This study aims to enhance the optical and electronic properties of g-C₃N₄ through carbon doping, morphological changes, chemical functionalization, and heterojunction formation, resulting in improved photocatalytic performance. In this study, kapok fiber was used as both a carbon doping source as well as a template for the microtubular structure by using the calcination method. Moreover, heterostructure formation between C-doped g-C₃N₄ (CCN) and polyaniline (PANI) was prepared through an in-situ oxidative polymerization reaction in the presence of additional chemical functionalization to further enhance the chemical intact between CCN and PANI. A comprehensive examination of the material's structural and textural characteristics, along with its crystallinity, chemical composition, optical properties, and charge carrier mobility, was conducted using various advanced characterization techniques. The results indicate that the additional functionalization has promoted the heterostructure formation with superior charge separation behaviour and light absorption capability compared to pristine photocatalysts. This enhanced photocatalytic functionality has contributed to the highest hydrogen peroxide production, 3922 μM g⁻¹ h⁻¹, which are 2.0, 4.2, and 5.6-fold over the CCN, PANI, and g-C₃N₄, respectively. Together with the advantageous band alignment, the strong interfacial contacts provide efficient electron-hole separation, which results in enhanced photocatalytic performance. In conclusion, an essential aspect of designing highly efficient photocatalysts for the future involves the creation of interconnected heterojunctions characterized by CCN microtubular structure and optimal growth of PANI within the heterojunction nanoarchitecture. The PANI/CCN structure, which forms a highly ordered photocatalyst, is believed to offer significant potential for practical photocatalytic applications.

Keywords: C-doped g-C₃N₄; Chemical functionalization; Nanoarchitecture; Heterojunction; H₂O₂ production

PHOTOCATALYTIC INTEGRATED CARBON CAPTURE AND UTILIZATION (ICCU) APPROACH FOR CONVERSION OF CO₂ TO METHANOL IN AMINE SOLUTION OF ACID GAS REMOVAL UNIT (AGRU)

Xin Hong Tai^a, Masniroszaim M Zain^a, Syafiq Bt M Saleh^a

^aCarbon Capture, Utilization & Storage (CCUS), R&D Department, PETRONAS Research Sdn. Bhd.,
Kawasan Institusi Bangi, 43000, Kajang, Selangor, Malaysia.

*Corresponding author: tai.xinhong@petronas.com

Abstract

Conventional CO₂ utilization methods are typically complex and expensive, primarily due to the need for capturing, purifying, storing, and transporting the CO₂ feedstock before it can be used. Recently, an alternative strategy known as Integrated Carbon Capture and Utilization (ICCU) has gained attention. This approach enables the direct use of CO₂ at the point of capture, such as in an acid gas removal unit (AGRU). In this study, we propose a novel ICCU technique in which CO₂ absorbed in an amine-based solvent is directly converted into methanol via photocatalysis. A magnesium-doped titanium dioxide (Mg-TiO₂) photocatalyst was prepared using a one-pot hydrothermal synthesis method. The resulting photocatalyst was characterized through XRD, UV-Vis spectroscopy, BET surface area analysis, and XPS. After 24 hours of photocatalysis reaction, the Mg-TiO₂ photocatalyst produced a methanol yield 2.4 times greater than that of pure anatase TiO₂. Additionally, the Mg-TiO₂ catalyst showed strong recyclability, maintaining its photocatalytic activity for up to six cycles. The improved performance is attributed to the magnesium dopant, which enhanced CO₂ adsorption and reduced charge carrier recombination. After 144 hours of photocatalysis, the amine solution retained most of its alkalinity, suggesting good preservation of the solvent's integrity. Interestingly, 8% of the captured CO₂ was released from the amine after 144 hours, indicating that the photocatalytic system functions as a dual-purpose setup—converting CO₂ into methanol while partially regenerating the amine's CO₂ capture capacity. To our knowledge, this is the first reported ICCU approach utilizing photocatalysis.

Keywords: CCUS, ICCU, Photocatalysis, amine, methanol

AMMONIA SYNTHESIS MECHANISM OVER RUTHENIUM-BASED CATALYSTS UNDER HIGH-PRESSURE REACTION CONDITIONS

Shuai Wang^{a,*}

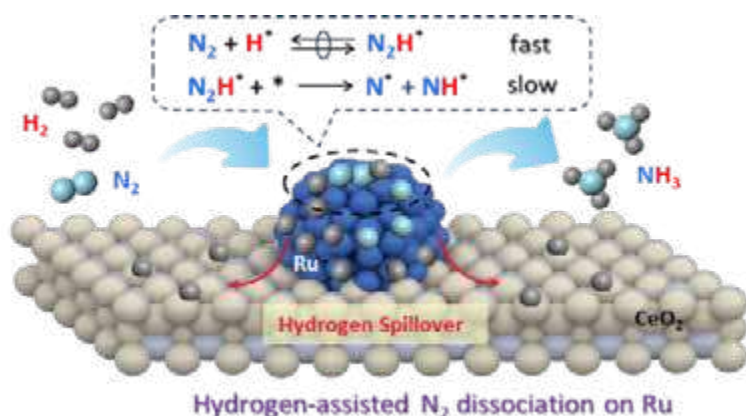
^aXiamen University

*Corresponding author: shuaiwang@xmu.edu.cn

Abstract

Understanding the roles of co-adsorbates on crowded catalytic surfaces is critical to optimizing industrial catalysts that are generally employed under high-pressure conditions. For ammonia synthesis from N₂ hydrogenation (i.e., the Haber-Bosch process), it is well-known that supported Ru catalysts tend to be highly covered by atomic H species, while the impact of these H species on N₂ activation is still in controversy. Herein, kinetic assessment, isotopic labelling experiments, and *in-situ* spectroscopic characterization were combined to investigate the mechanism of ammonia synthesis on Ru/CeO₂ catalysts with their structure tuned via thermal treatments. Our experimental approaches reveal that the dominant H* surface species limit the availability of vacant Ru sites for the widely-proposed direct N₂ dissociation route, but instead, lead to the prevalence of H-assisted N₂ dissociation route with the N-N cleavage in N₂H* intermediates as a kinetically-relevant step. Effects of Ru particle size and Ru-CeO₂ interaction on the catalytic activity were kinetically deconvoluted in accordance with this H-assisted mechanism, unveiling their decisive influences on the intrinsic activity and surface coverage, respectively. Driven by these fundamental insights gained from the working conditions, superior ammonia formation rates were achieved for supported Ru catalysts via optimizing Ru particle size and metal-support interaction collaboratively.

Keywords: H-assisted N₂ dissociation, structure-activity relationship, Ru-based catalyst, hydrogen spillover, kinetics



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PLASMA CATALYSIS FOR EFFICIENT CO₂ CONVERSION

Hao Zhang^{a,*}, Yanhui Long^a, Kaiyi Wang^a, Xiaodong Li^a, Jianhua Yan^a

^a State Key Laboratory of Clean Energy Utilization, Zhejiang University, Hangzhou 310027, China.

*Corresponding author: zhang_hao@zju.edu.cn

Abstract

Atmospheric plasma processes have risen to the forefront as a promising avenue for CO₂ conversion. In this work, our recent efforts on improving the efficiency of CO₂ conversion into clean CO by plasma and plasma catalysis will be presented.

1. By enhancing the gas treatment in the plasma area, e.g., via optimization of the injector nozzle, use of a quadrangular cover, and development of a magnetically enhanced gliding arc, the CO₂ conversion and energy efficiency can be both improved to some extent¹.
2. Furthermore, we introduce an innovative in-situ gas sampling technique, enabling 2D spatial mapping of product compositions, experimentally confirming for the first time the substantial limiting effect of CO recombination reactions in the afterglow region. We then constructed a comprehensive 2D model that allows for spatial reaction rates analysis incorporating crucial reactions.² 3) Significant enhancement in the performance is then achieved by inhibiting the recombination reaction, through e.g., cooling the reactor, and introduction of biochar to allow for the reverse Boudouard reaction (CO₂+C→ 2CO).³ 4) Very interestingly, we propose a novel Plasma Chemical Looping CO₂ Splitting (PCLCS) approach that integrates a rotating gliding arc plasma with zirconium-doped ceria (Ce_xZr_{1-x}O₂, x=0.1- 0.5) oxygen carriers (OCs), enabling highly efficient CO₂ conversion (84%) into O₂-free CO at mild temperature of only 320 °C, demonstrating a robust synergy between plasma and OCs.⁴ 5) Also, we propose a plasma TiO₂ photocatalytic strategy that produces a strong plasma-catalysis synergy for CO₂ splitting (only in the in-plasma catalysis mode), improving remarkably the reaction performance.⁵ These efforts provide critical clues for further enhancement of CO₂ activation in the promising plasma processes.

Keywords: CO₂ conversion, plasma, plasma catalysis, plasma chemical looping

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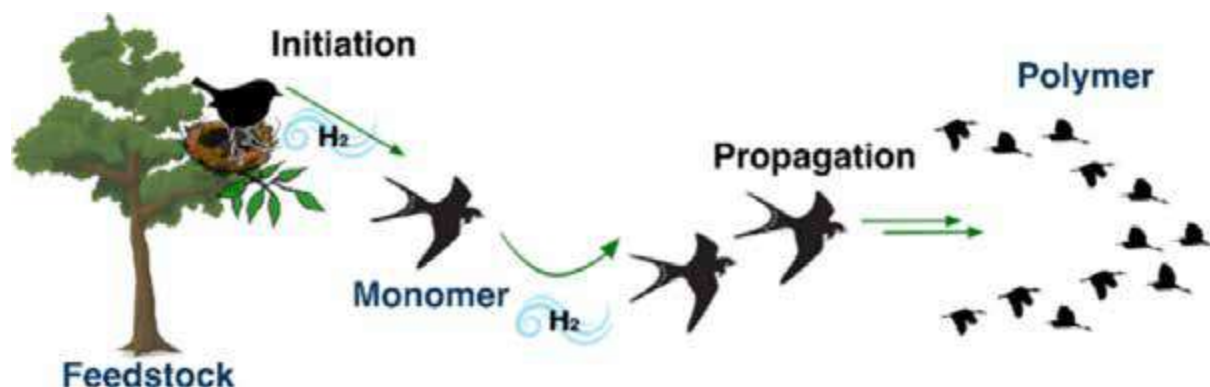
DEHYDROGENATIVE AND HYDROGENATIVE CATALYSIS FOR THE SYNTHESIS AND RECYCLING OF POLYMERS

Amit Kumar

School of Chemistry, University of St. Andrews, KY169ST, Email: ak336@st-andrews.ac.uk.

Abstract

The development of sustainable methods for the closed-loop production and recycling of plastics is an important challenge of the current times. Reactions based on catalytic (de)hydrogenation are atom-economic and sustainable routes for organic transformations. This lecture will discuss the application of homogeneous (de)hydrogenative catalysis for the synthesis and degradation of plastics such as nylons, polyureas, polyureaurethanes, polyethylenimines, polyketones, and polyesters.¹



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PREPARATION OF FURAN PLATFORM MOLECULES FROM (HEMI) CELLULOSE AND THEIR DOWNSTREAM CONVERSION

Xianhai Zeng^{a,b,*}, Shaoyu Yuan^a

^aCollege of Energy, State Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361102, China.

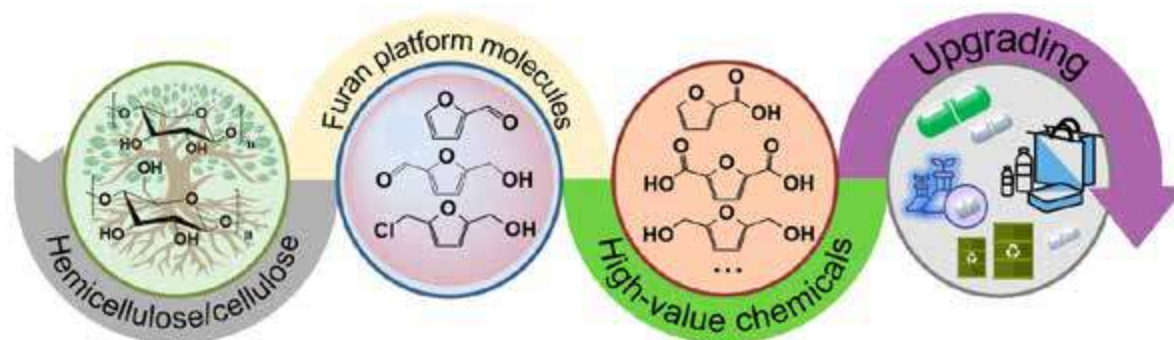
^bFujian Engineering and Research Center of Clean and High-valued Technologies for Biomass, Xiamen Key Laboratory of Clean and High-valued Utilization for Biomass, Xiamen University, Xiamen 361102, China.

*Corresponding author: xianhai.zeng@xmu.edu.cn

Abstract

The preparation and utilization of biomass-derived platform molecules to replace traditional non-renewable organic synthetic pathways based on fossil resources is important for the energy transition and sustainable development goals¹. Furan-based platform molecules derived from (hemi)cellulose, can be catalysed into a variety of bio-based chemicals, fuels and polymer monomers, which is an important means of sustainability and green decarbonization of chemicals, fuels and materials^{2,3}. Based on the accumulation by the author's group, this presentation reviews the conversion of (hemi)cellulose into furan platform molecules and its downstream high-value conversion and utilization ways. It mainly includes the preparation of furan platform molecules by catalytic pyrolysis and acid catalysis from (hemi)cellulose and their further conversion into a variety of high value-added products by catalytic hydrogenation/oxidation/ammonification. Finally, the opportunities and challenges in the preparation of furan platform molecules from (hemi)cellulose and their downstream conversion are discussed.

Keywords: (Hemi) cellulose, Furan platform molecule, Catalysis, Conversion of biomass



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RATIONAL DESIGN OF ELECTROCATALYSTS FOR EFFICIENT OXYGEN EVOLUTION TOWARD CARBON-NEUTRAL HYDROGEN PRODUCTION

Hyeyoung Shin^{a,*}

^aChungnam National University.

*Corresponding author: shinhy@cnu.ac.kr

Abstract

Electrochemical water splitting represents a key technology for carbon-neutral hydrogen production, yet its practical implementation is hindered by the sluggish kinetics of the oxygen evolution reaction (OER). To overcome this limitation, we aim to establish rational design strategies for highly active OER electrocatalysts based on fundamental mechanistic insights. In this work, density functional theory (DFT) calculations were employed to systematically investigate the OER pathway on nickel oxyhydroxide (NiOOH) and a series of transition metal-doped derivatives. By analyzing the adsorption free energies of critical OER intermediates, we elucidate how dopant-induced modifications in the local electronic environment influence the energetics of individual reaction steps. The results reveal that specific dopants promote more favorable charge redistribution and intermediate stabilization, leading to reduced theoretical overpotentials. This mechanistic understanding highlights the critical role of electronic structure engineering in enhancing catalytic performance. The findings provide a theoretical framework for guiding the composition and design of advanced nanocatalysts, contributing to the development of efficient and scalable water electrolysis systems aligned with carbon-neutral energy goals.¹⁻⁴

Keywords: oxygen evolution reaction, nickel oxyhydroxide, density functional theory, electrocatalyst design, carbon-neutral hydrogen production

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PHOTOELECTROCHEMICAL ACTIVITY OF Fe_2O_3 /NICKEL-FOAM PHOTOANODE UNDER ELECTROLYTE BIAS FOR WATER SPLITTING

Alia Khairani Mat Nasir^a, Shaarvin Elangovan^b, Lorna Jeffery Minggu^{b,*}, Rozan Mohamad Yunus^b,
Mohamad Azuwa Mohamed^{a,b}, Mohammad B. Kassim^{a,b}

^aDepartment of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600,
UKM Bangi, Selangor, Malaysia.

^bFuel Cell Institute, Universiti Kebangsaan Malaysia, 43600, UKM Bangi, Selangor, Malaysia.

*Corresponding author: lorna_jm@ukm.edu.my

Abstract

Direct hydrogen production via photoelectrochemical (PEC) water splitting represents a promising pathway toward sustainable, renewable, and clean hydrogen generation. However, current PEC system often requires additional energy input beyond what is provided by solar energy alone. In this study, strategies involving pH bias and the use of donors were investigated to enhance the photovoltage for PEC water splitting. The photoanode was prepared by electrodeposition of iron hydroxide on nickel foam (NF) and followed by annealing to form Fe_2O_3 /NF. Different annealing temperatures were studied to determine the best condition for PEC performance. The photoanodes were characterized using SEM, EDS, XRD, and UV-Vis spectroscopy. PEC activity was initially evaluated in a single-cell configuration to assess the effect of annealing temperature. Subsequently, the photoanode was tested in an H-cell configuration, where the anode and cathode compartments were separated by a membrane and filled with alkaline and acidic electrolytes, respectively. The optimal annealing temperature was found to be 400 °C, yielding the highest activity. The addition of donors in the anode compartment significantly reduced the onset potential. The combined effect of pH bias and donors enabled PEC- assisted water splitting without the need for external electrical connection.

Keywords: Fe_2O_3 , Nickel foam, electrolyte bias, Photoelectrochemical, Water splitting

MULTI-SITE SYNERGISTIC CATALYSIS FOR DIRECTED CONVERSION

Qing Han*

Laboratory of Advanced Materials, Fudan University, Shanghai, China

*Email: qhan@fudan.edu.cn

Abstract

Harnessing renewable energy (e.g., solar) to convert abundant small molecules (O_2 , CO_2 , CH_4) into high-value chemicals under mild conditions represents a pivotal technology for clean energy storage and green economy development. We propose a multi-site synergistic catalysis strategy to achieve highly active and selective molecular activation: (1) In covalent organic frameworks, engineered fluorine-olefin proximity creates p- π conjugation that induces spin polarization to activate triplet O_2 into $^1O_2$, enabling 94% selective H_2O_2 production; (2) A “pre-locking/nanoconfined polymerization” approach yields electron-delocalized triangular Cu_3 sites (Cu(I)-dominant) that facilitate asymmetric C-C coupling between bridge- and atop-adsorbed CO, directing the pathway through $^*CHCHOH$ intermediate to achieve 99% ethanol selectivity; (3) Au-oxygen vacancy-Bi ternary sites promote $\bullet OH$ -mediated CH_4 activation to $\bullet CH_3$ while scavenging excess $\bullet OH$ in situ, optimizing the $\bullet CH_3/\bullet OH$ ratio for 90% selective ethanol production via C-C coupling.

Keywords:

photocatalysis; active sites; O_2 reduction reaction; CO_2 reduction reaction; CH_4 oxidation reaction

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SCALABLE SYNTHESIS OF EARTH-ABUNDANT CATALYSTS VIA MAGNETRON SPUTTERING FOR ELECTROCHEMICAL WATER SPLITTING

Farid Attar and Siva Karuturi*

School of Engineering, The Australian National University, Canberra ACT 2601, Australia

**Corresponding author: siva.karuturi@anu.edu.au*

Abstract

Green hydrogen production via water electrolysis is an attractive solution to decarbonise energy systems, but its commercial adoption is hindered by the cost and scalability challenges associated with noble metal-based catalysts. This work investigates the scalable fabrication of earth-abundant, Ni-based catalysts using magnetron sputtering for both oxygen and hydrogen evolution reactions (OER and HER). The direct synthesis of Ni₃N/Ni catalysts enriched with nitrogen vacancies via one-step magnetron sputtering demonstrated low overpotentials and excellent stability, highlighting the potential of sputtered catalysts for both standalone and integrated solar-fuel systems. Further, a trimetallic NiFeMoN catalyst was synthesised via one-step co-sputtering and optimised through design of experiments (DOE), response surface methodology (RSM), and ANOVA. The optimised catalyst demonstrated high OER activity with an overpotential of 216 mV at 10 mA cm⁻² and prolonged stability over seven days. For HER, a NiMoC catalyst was developed using a triple-target co-sputtering process at room temperature, achieving overpotentials of 26 mV (alkaline) and 42 mV (acidic) with stable operation up to 10 days (alkaline) and 70 hours (acidic). The enhancements arise from Mo₂C and NiMo active sites and improved conductivity and stability from disordered and graphite-like carbon. Integrated into a zero-gap electrolyser, NiMoC enables cell voltages of 1.87 V at 1 A cm⁻². These results establish magnetron sputtering as a viable route to scalable, high-performance catalyst fabrication for industrial water splitting applications.

Keywords: Magnetron sputtering, Earth-abundant catalysts, Multi-metallic catalysts, Water electrolysis, Room temperature synthesis

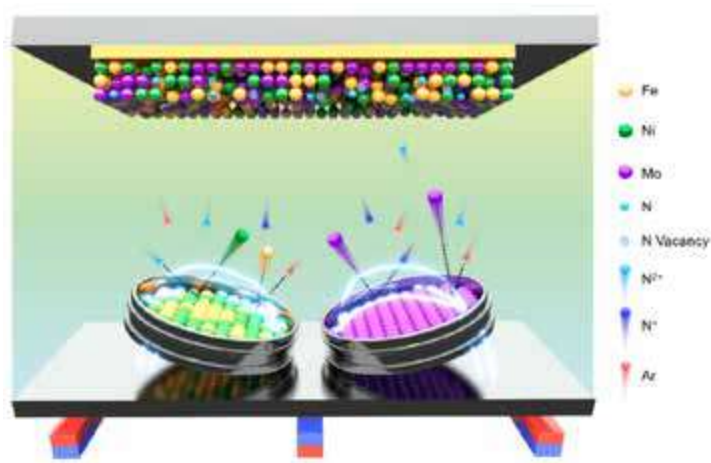


Figure 1. Schematic of NiFeMoN deposition by magnetron co-sputtering method.

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TAILORING ELECTROLYTE FORMULATIONS FOR GREEN AMMONIA ELECTROPRODUCTION FROM NITROGENOUS SPECIES

Sara Garcia-Ballesteros^{a,*}, Noemi Pirrone^a, Lorenzo Sibella^a, Anna Mangini^a, Federico Bella^a,

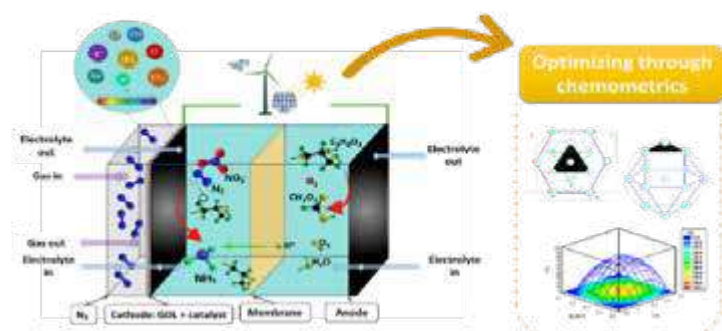
Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 - Turin, Italy.

**Corresponding author: sara.garcia@polito.it*

Abstract

Ammonia is a critical commodity for the global economy, primarily used in fertilizers production and increasingly considered as a potential carbon-free energy carrier. However, its conventional synthesis via the Haber-Bosch process for ammonia synthesis is highly energy-intensive, relying on fossil fuels and contributing to approximately 2% of global energy consumption and significant CO₂ emissions. [1] As a sustainable alternative, green ammonia production via electrochemical nitrogenous species reduction has emerged as a promising approach. [2] A key factor influencing the efficiency of this process is the electrolyte, which plays a fundamental role in determining reaction kinetics, selectivity, and overall yield. In fact, it is well known that the electrolyte composition and properties can impact the process outcome by several orders of magnitude [3]. Despite its importance, optimizing electrolytes for ammonia electroreduction remains a major challenge. In this context, our research group has dedicated significant efforts to advancing electrolyte design and understanding its influence, along with other operational parameters, on green ammonia production. For example, the electrochemical nitrate reduction reaction (E-NO₃RR) was tailored for a MoS₂ catalyst, a material well known for its activity toward the competing hydrogen evolution reaction (HER). To systematically analyse the effects of different operating conditions, we employed design of experiments (DoE) and response surface methodology (RSM). Results identified applied potential and salt concentration as the key parameters controlling process efficiency. Through this approach, we successfully increased the system efficiency from 10% to 80%. Additionally, the influence of various anions and cations commonly found in real water sources was investigated to move toward more realistic application scenarios. Regarding the electrochemical nitrogen reduction reaction (E-NRR), our ongoing research explores, among other strategies, the use of a glycerol-water mixture as an electrolyte solvent to enhance N₂ solubility and mitigate HER competition, ultimately improving nitrogen reduction selectivity and efficiency.

Keywords: green ammonia electrosynthesis, nitrogen reduction reaction, nitrates reduction reaction, chemometrics



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CATALYTIC TRANSFORMATION OF CELLULOSE USING BASIC COPPER CARBONATE PREPARED *VIA* SUPERCRITICAL CO₂ ANTISOLVENT PRECIPITATION

Kok-Hou Tan^{a,*}, Po-Wen Chung^b, Stuart H. Taylor^a

^a*Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Translational Research Hub, Maindy Road, Cardiff CF24 4HQ, UK.*

^b*Institute of Chemistry, Academia Sinica, 128 Academia Road, Section 2, Nankang, Taipei 11529, Taiwan.*

**Corresponding author: TaylorSH@cardiff.ac.uk*

Abstract

Global warming and climate change resulting from industrialization and fossil fuel consumption are threatening the survival of flora and fauna on Earth. Switching to renewable resources is deemed required to mitigate their negative impacts and promote the sustainability of life. To achieve sustainable consumption and production as outlined in the United Nations Sustainable Development Goal No. 12, the utilization of agricultural waste as a renewable feedstock for chemical manufacturing is highly desirable as the industry release more than 2 Gt of greenhouse gases per annum to the atmosphere.¹ Particularly, the transformation of lignocellulosic components of agricultural waste into platform chemicals has been identified as an economically viable option and an efficient catalyst is the key to the production of bio-based chemicals at a practical yield. In this study, basic copper carbonate catalysts were prepared using the supercritical CO₂ antisolvent (SAS) precipitation method, which permitted rapid formation and drying of catalysts.² The as-synthesized copper carbonate catalyst was found to have a larger specific surface area and pore volume than its co-precipitated counterpart. XRD analysis showed that the resulting carbonate catalysts comprised of malachite structure with their crystallinity increased with precursor metal concentration. These candidates were evaluated for their activity in catalytic depolymerization of cellulose under a CO₂ atmosphere. Further studies were conducted to determine the kinetic and reaction mechanism of this novel metal carbonate-catalyzed cellulose depolymerization reaction. The results showed that copper carbonate is capable of breaking cellulose into mono- and oligosaccharides, such as glucose and cellobiose, at moderate temperature (150 °C) and high CO₂ pressure (30 bar).

Keywords: Renewable source, Transition metal carbonate, Supercritical CO₂, Hydrothermal, Heterogeneous catalysis

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P-METHOXY SUBSTITUENTS IN COBALT PHTHALOCYANINE FOR EFFICIENT ELECTROCHEMICAL CO₂ REDUCTION

Mengxin Liu,^a Yuming Wu,^a Xiuping Liao,^a Oliver J. Conquest,^{b,c} Catherine Stampfl,^{b,c}
and Yijiao Jiang,^{a*}

^a School of Engineering, Macquarie University, Sydney, NSW 2109, Australia

^b School of Physics, The University of Sydney, New South Wales 2006, Australia

^c The University of Sydney Nano Institute, The University of Sydney, New South Wales 2006, Australia

*Corresponding author: yijiao.jiang@mq.edu.au

Abstract

Electrochemical CO₂ reduction to CO (CO₂RR) using molecular catalysts is a promising strategy for sustainable fuel and chemical production. Cobalt phthalocyanine (CoPc) has emerged as a leading candidate owing to its structural robustness and tunable electronic properties. Here, we systematically investigate the influence of methoxy substitutions at the para and ortho positions on CoPc activity and stability. The results demonstrated that para-CoPc(OMe)₈ significantly outperformed ortho-CoPc(OMe)₈ and unsubstituted CoPc, achieving a FE_{CO} of 95 ± 2.4% at −1.05 V vs. NHE and exhibiting excellent operational stability. Electrochemical analyses (CV, LSV, TOF) indicate that para-substitution enhanced the density of electrochemically active sites and promoted electron transfer kinetics. Density functional theory (DFT) calculations reveal that para-methoxy groups increase electron density at the cobalt center, reduce steric hindrance, and improve active site accessibility. These synergistic electronic and structural effects facilitate CO₂ adsorption and suppress catalyst deactivation. This work highlights the critical role of substituents positioning and provided a rational design strategy for next-generation molecular CO₂RR catalysts.

Keywords: CO₂ reduction, cobalt phthalocyanine, methoxy substitutions, stability

PLURONIC F127-ASSISTED SYNTHESIS OF MESOPOROUS FENC AS ADVANCED ELECTROCATALYSTS FOR OXYGEN REDUCTION REACTION

Muhammad Amirul Aiman Abdul Rani^a, Muhamad Amirul Aiman Mohd Nor^a, Wai Yin Wong^{a*},
Kee Shyuan Loh^a, Mohd Shahbudin Bin Mastar @ Masdar^a, Nabila A Karim^a

^a Fuel Cell Institute, Universiti Kebangsaan Malaysia, Bangi 43600, Selangor, Malaysia

*Corresponding author: waiyin.wong@ukm.edu.my

Abstract

The development of non-platinum group metal (PGM) catalysts for the oxygen reduction reaction (ORR) is essential for lowering the cost of proton exchange membrane fuel cells. This study explores a soft-template strategy to synthesize an atomically dispersed iron-doped nitrogen-carbon (FeNC) catalyst with a core-shell structure. A surfactant-assisted metal-organic framework (MOF) approach was employed, where the interaction between Pluronic F127 and Fe-doped zeolitic imidazolate framework (ZIF-8) nanocrystals induced a confinement effect. This effect, influenced by the mass ratio of surfactant to 2-methylimidazole (2-mIm), played a crucial role in suppressing the aggregation of iron atomic sites during thermal activation while preserving the microporous structure of ZIF-8, thereby enhancing catalytic activity. The study found that the optimal mass ratio of F127 to 2-mIm significantly improved the active site density. The FeNC-F127-m1 catalyst exhibited outstanding ORR performance in acidic media under nitrogen environment, achieving an onset potential (E_{onset}) of 0.92 V (vs. RHE) and a half-wave potential ($E_{1/2}$) of 0.774 V (vs. RHE). Furthermore, it delivered a high diffusion-limiting current density ($j_L = 5.568 \text{ mA/cm}^2$), surpassing conventional Fe-N-C catalysts ($j_L = 4.3 \text{ mA/cm}^2$) and approaching the activity of commercial Pt/C catalysts. This enhancement can be attributed to the improved exposure of active sites and accelerated electron transfer kinetics. These findings highlight the effectiveness of surfactant-assisted MOF synthesis in fine-tuning Fe-N-C catalysts by optimizing the surfactant-to-2-mIm mass ratio, offering a promising pathway for cost-effective and high-performance ORR electrocatalysts in fuel cell applications.

Keywords: Oxygen reduction reaction; FeNC; surfactant; F127; proton exchange membrane fuel cell.

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PROBING THE INDEPENDENT EFFECTS OF PYROLYSIS TEMPERATURE AND REDUCING GAS TREATMENT ON ACTIVE-SITE FORMATION IN Pt, Fe-N-C INTERMETALLIC CATALYST FOR ACIDIC OXYGEN REDUCTION REACTION

Muhamad Amirul Aiman Mohd Nor^a, Muhammad Amirul Aiman Abdul Rani^a, Wai Yin Wong^{a*},
Kee Shyuan Loh^a, Long Kean Lim^a, Siti Hasanah Osman^a, Foo Thye Choo^b

^aFuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.

^bMalaysian Nuclear Agency, Bangi, Kajang, Selangor 43000, Malaysia

*Corresponding author: waiyin.wong@ukm.edu.my

Abstract

The oxygen reduction reaction (ORR) at proton exchange membrane fuel cell (PEMFC) cathodes requires efficient electrocatalysts to overcome kinetic limitations, with Pt-based materials remaining the benchmark. Recently, Pt,Fe-N-C catalysts have emerged as promising alternatives, offering enhanced activity and durability through the formation of PtFe intermetallic structures and nitrogen-coordinated active sites. This study examines how two critical synthesis parameters independently influence active-site formation in Pt,Fe-N-C catalysts: (1) first-step pyrolysis temperature and (2) application of H₂/N₂ reducing gas at different synthesis stages. Catalysts were prepared through Pt impregnation of a Fe-containing MOF precursor followed by controlled two-step pyrolysis, systematically varying the first-step temperature while maintaining the second step at 900°C. Parallel experiments investigate the role of H₂ introduction timing (first step only, or both steps) in precursor reduction and intermetallic formation. Electrochemical characterization reveals how these processing variables affect catalyst structure and ORR performance. The findings provide fundamental insights into the separate roles of thermal and chemical treatment in PtFe-N-C active-site engineering, contributing to the development of more efficient PEMFC cathode catalysts.

Keywords: Oxygen reduction reaction; gas treatment; active sites; proton exchange membrane fuel cell.

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POTASSIUM-DRIVEN PATHWAY MODULATION IN CO₂ HYDROGENATION: TUNING ETHANOL AND LIQUID FUELS SYNTHESIS OVER FECUAL CATALYST

Wenjie Xiang^a, Shuhei Yasuda^a, Noritatsu Tsubaki^{a*}

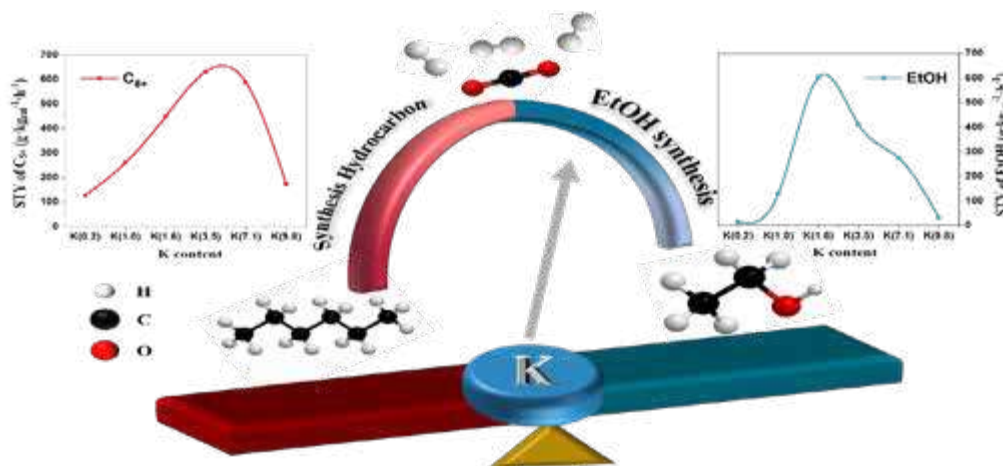
^aUniversity of Toyama

*Corresponding author: tsubaki@eng.u-toyama.ac.jp

Abstract

The hydrogenation of CO₂ into value-added chemicals and fuels represents a viable strategy for carbon recycling and sustainable energy production. This study investigates the effect of potassium (K) loading on FeCuAl catalysts, specifically focusing on tuning the selectivity between ethanol and C₅₊ hydrocarbons. A series of K(x)/FeCuAl catalysts were synthesized using a co-precipitation method followed by controlled K impregnation, allowing precise modulation of catalytic properties. The results demonstrate that K loading plays a pivotal role in modifying the reaction pathway by influencing CO₂ adsorption, CO formation, and carbon chain growth via C–C coupling. At an optimal K loading of 1.6 wt%, the catalyst exhibited the highest ethanol space-time yield (STY) of 603 g_{AcH}/kg_{cat} h⁻¹, whereas increasing K loading to 3.5 wt% shifted the product distribution toward C₅₊ hydrocarbons, achieving a peak STY of 632 g_{fuel}/kg_{cat} h⁻¹. Comprehensive characterizations, including X-ray photoelectron spectroscopy (XPS), Mössbauer spectroscopy, and in-situ diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy, revealed that K enhances surface alkalinity, stabilizes Fe carbides, and alters the electronic environment of active sites, ultimately governing product selectivity. The study provides mechanistic insights into the pathway regulation in CO₂ hydrogenation and offers a tunable catalytic strategy for optimizing the selective production of liquid fuels and oxygenates.

Keywords: CO₂ hydrogenation, Fe-based catalyst, K loading, C₅₊ hydrocarbons, ethanol



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CATALYST SHAPING FORMULATION FOR CATALYTIC REACTIONS IN FIXED BED REACTOR

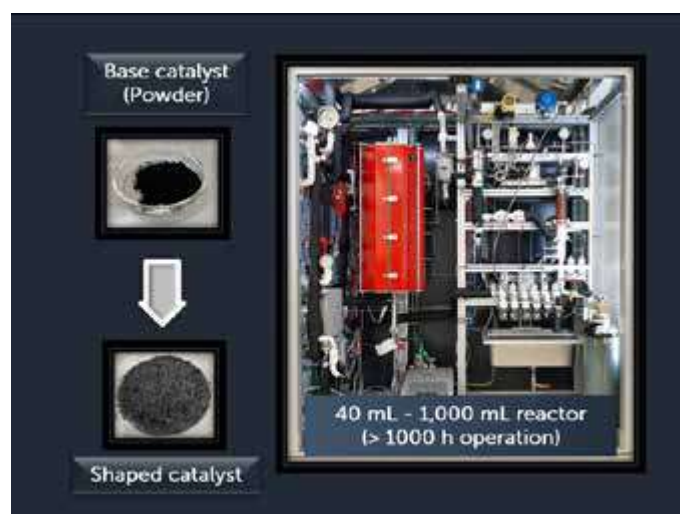
Nik Nik M Adnan^{a,*}, Suhaimi Abd Razak^a, Ashraf Zin Zawawi^a, Jamali Basar^a
^aPETRONAS

*Corresponding author: nmsyafiq.nmadnan@petronas.com

Abstract

It is undeniable that one of the major hurdles to successfully scale up a refinery catalyst for commercialisation is the catalyst shaping into extrudates, particularly for trickle bed reactor applications¹. Typically, the catalyst is deployed in the form of extrudates that mechanically can withstand severe reaction conditions throughout the catalyst lifespan. PETRONAS has recently developed a novel catalyst that is composed of molybdenum sulphides with structural carbon for hydrodeoxygenation reaction of lipid materials into hydrocarbon. In the effort to scale up the catalyst for commercialisation, the catalyst powder needs to be shaped into extrudates of suitable size, to fit into a lab and pilot scale continuous flow reactors. However, the catalyst is unique, composed of hard-to-shape materials that include molybdenum sulphides and structural carbon that is intrinsic properties of the catalyst. Limited information exists in the public domain on shaping of such material, unlike conventional oxide catalysts² that are easier to handle and well known to the industry. Following extensive screening and optimisation, the team has successfully developed a durable extrudates based on boehmite binder formulation. The shaped catalyst displayed excellent mechanical properties, as indicated by side crush strength and attrition tests, matching commercial catalyst physical characteristics. The catalytic activity of the extrudates remained excellent, achieving full conversion throughout the test and was not hampered by dilution of active materials in the formulation. The mechanical strength of the catalyst was further exemplified with continuous operation of up to 1000h in a pilot scale continuous flow reactor.

Keywords: Catalyst shaping; hydrodeoxygenation process; catalytic reactions, molybdenum disulphide



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ELECTROCATALYTIC CO₂ REDUCTION USING LANTHANOID-DOPED CATALYSTS

WeiQi Liu*

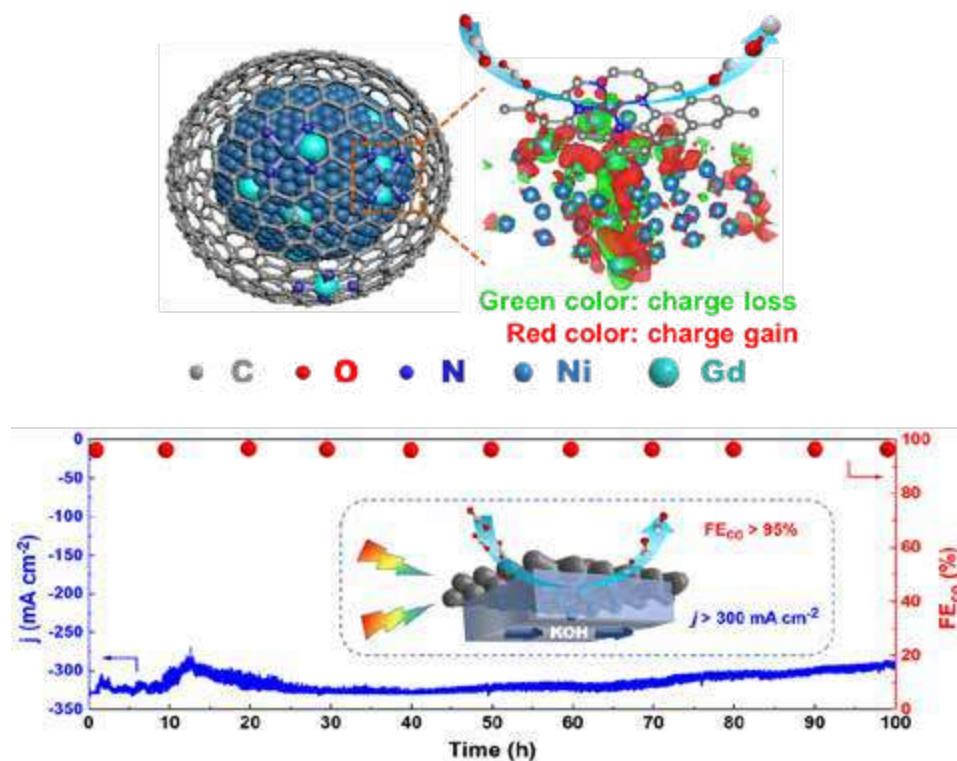
MOE Key Laboratory of Coal Processing and Efficient Utilization, School of Chemical Engineering and Technology, China University of Mining and Technology, 1 Daxue Road, Xuzhou, Jiangsu, 221116, China

*Corresponding author: weiqi.liu@cumt.edu.cn

Abstract

Electrocatalytic CO₂ reduction (ECR) is considered to be one of the most promising approaches for achieving the recycling CO₂ due to its advantages such as mild reaction conditions, simple system, and utilization of renewable energy. The first-row transition metals, which are inexpensive and widely available, have been extensively studied in the field of ECR. However, their directionally localized 3d orbitals make it difficult to provide a large number of electrons for coupling CO₂/intermediates, which leads to their low ECR activity. The loose 4f and unfilled 5d orbitals of lanthanoid endow it with a strong spin-orbital coupling effect, which enables it to effectively regulate the electronic structure of other metals. Consequently, we prepared a lanthanoid Gd-doped Ni-based catalyst using self-assembly method to optimize the electronic structure of the Ni active sites and enhance the ECR performance of the catalyst. It is shown that the polarization effect of Gd atoms can promote the movement of electrons in the 3d orbitals of Ni active sites towards higher energy levels outside the nucleus, which significantly increases the intrinsic activity of the Ni active sites. The as-resulted highly active Ni sites exhibit strong adsorption strength for CO₂/*COOH, remarkably lowering the energy barrier for the formation of *COOH and promoting the generation of CO. Therefore, the lanthanoid-doped catalyst shows a high CO selectivity (90%), a large current density (308 mA cm⁻²), and a superbly electrochemical stability (100 h). This work provides a new research approach for improving the ECR performance of transition metals by doping lanthanoid.

Keywords: electrocatalytic CO₂ reduction, lanthanoid, electronic structure



RESEARCH ON THE ELECTROCATALYTIC MECHANISM OF NITROGEN/OXYGEN-RELATED SPECIES ON CARBON-BASED MATERIAL INTERFACE

Peiyao Bai^{a*}

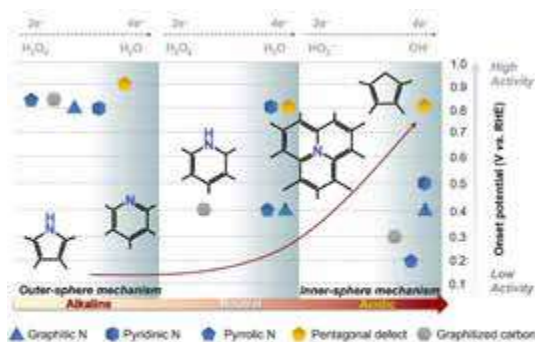
^a School of Chemical Engineering and Technology, China University of Mining and Technology

*Corresponding author: Peiyao Bai (peiyao.bai@cumt.edu.cn)

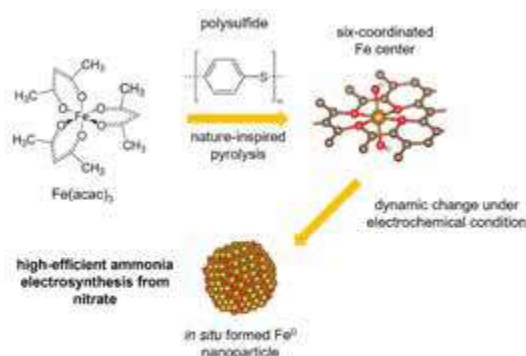
Abstract

Carbon-based catalysts have garnered significant attention for their potential applications in electrocatalysis, particularly in oxygen/nitrogen-related electrochemical processes. Understanding the molecular interface reaction mechanisms involving nitrogen and oxygen species is crucial for optimizing their catalytic performance. This study aims to elucidate the electrocatalytic interface reaction mechanisms of nitrogen/oxygen species on carbon-based catalysts, focusing on how these mechanisms influence the overall catalytic efficiency and selectivity in oxygen reduction reactions (ORR) and nitrate reduction reactions (NO₃RR). A combination of experimental and theoretical approaches was employed. Experimental methods included the synthesis of heteroatom-doped porous carbons using dry-chemistry techniques and the preparation of iron-based catalysts with dynamic sites for NO₃RR. Characterization techniques such as X-ray fine adsorption spectroscopy (XAFS), scanning transmission electron microscopy (STEM), surface-enhanced infrared absorption spectroscopy (SEIRAS), ab-initio molecular dynamics (AIMD) and density functional theory (DFT) simulations were used to analyze the catalyst structures and their reaction mechanisms. Nitrogen-doped carbons exhibited enhanced catalytic performance due to optimized micropore structures and synergistic effects between different nitrogen species. However, the real pH-universal active sites in nitrogen-doped carbon is pentagonal defect structure. Dynamic iron sites in the catalyst underwent a dissolution-migration-reduction process, forming Fe⁰ nanoparticles that facilitated the crossover mechanism, leading to high ammonia yield in NO₃RR. The study provides insights into the critical role of nitrogen and oxygen species in the electrocatalytic interface reactions of carbon-based catalysts. The findings highlight the importance of optimizing pore structures and doping configurations to enhance catalytic performance. Future work will focus on further optimizing these catalysts for practical applications in energy conversion and environmental remediation.

Keywords: Oxygen reduction reaction, Nitrate reduction reaction, Synergistic effect, Dynamic active site, Electrochemical interface mechanism.



Interfacial identification of the active sites in nitrogen-doped carbon for ORR



Interfacial dynamic active sites mechanism of the sulfur-doped carbon for NO₃RR

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HIGH-ENTROPY TRANSITION METAL DICHALCOGENIDE CATALYSTS FOR UREA OXIDATION

Hyojung Lim^a, Jinuk Choi^a, Uk Sim^{a,b,*}

^aKorea Institute of Energy Technology (KENTECH)

^bNEEL Sciences, Inc.

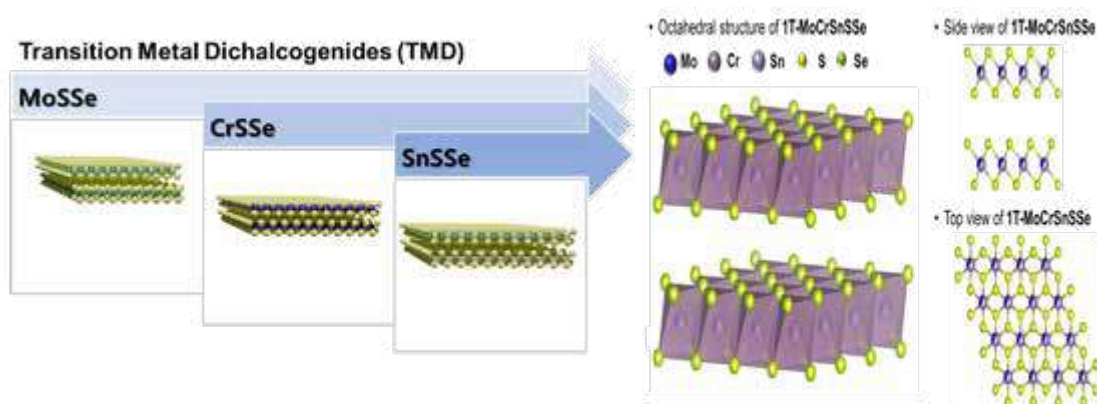
*Corresponding author: usim@kentech.ac.kr

Abstract

The urea oxidation reaction (UOR) is an energy-efficient alternative to the oxygen evolution reaction (OER), requiring only 0.37 V *vs.* RHE compared to OER (1.23 V *vs.* RHE). UOR enables both hydrogen production and wastewater treatment by utilizing urea, a common nitrogenous pollutant. Transition metal dichalcogenides (TMDs) have been studied as electrocatalysts due to their 2D structure and tunable properties.¹ However, conventional TMDs often exhibit limited activity and stability. High-entropy TMDs (HE-TMDs), composed of multiple transition metals and chalcogenides, improve catalytic performance through high configurational entropy and synergistic effects. In this study, a HE-TMD catalyst, MoCrSnSSe/rGO, was synthesized via a hydrothermal method. The catalyst achieved a configurational entropy of 1.65 R. The MoCrSnSSe/rGO catalyst demonstrated excellent UOR performance, achieving 10 mA cm⁻² at a low potential of 1.394 V *vs.* RHE in 1 M KOH with 0.33 M urea solution. The integration of high entropy, 2D structure, and multi-element synergy contributes to both activity and stability. This study demonstrates the potential of HE-TMDs as cost-effective UOR catalysts and provides a pathway toward sustainable and energy-efficient electrochemical systems.

Keywords: electrochemical urea oxidation, high-entropy transition metal dichalcogenide, high-entropy materials, transition metal dichalcogenide, water electrolysis

Graphic / Image



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CoNiCuRu/MWCNT CATALYST ACHIEVING 43.3% ENERGY EFFICIENCY FOR ELECTROCHEMICAL AMMONIA PRODUCTION FROM NITRATE

Jinuk Choi^{a,*}, Gyoung Hwa Jeong^{b,*}, Hyojung Lim^b, Uk Sim^c,

^a Hydrogen Energy Technology Laboratory, Korea Institute of Energy Technology (KENTECH), Jeonnam 58330, Republic of Korea.

^b Research Institute, NEEL Sciences, INC., Jeollanamdo 58326, Republic of Korea.

*Corresponding author: usim@kentech.ac.kr

Abstract

Ammonia (NH₃) plays a critical role in industries ranging from fertilizer production to hydrogen storage and clean energy applications. Traditionally, NH₃ is synthesized through the Haber-Bosch process, which operates under high temperature and pressure and heavily depends on fossil fuels, thereby generating considerable CO₂ and NO_x emissions¹. This raises significant concerns regarding environmental impact and sustainability.

Electrochemical nitrate reduction has emerged as an attractive alternative, enabling NH₃ synthesis under mild conditions with reduced energy input and greenhouse gas emissions. Notably, utilizing nitrate (NO₃⁻) as a nitrogen source simultaneously addresses water contamination issues by removing nitrate pollutants².

In this work, we report the development of a quaternary CoNiCuRu alloy catalyst supported on multi-walled carbon nanotube (MWCNT) electrochemical NH₃ synthesis from NO₃⁻ under for ambient condition. The CoNiCuRu/MWCNT catalyst demonstrates excellent catalytic activity, achieving a high ammonia production rate of 3.1 mg h⁻¹ cm⁻² and a Faradaic efficiency exceeding 90% at 0.1 V vs. RHE. A notable half-cell energy efficiency of 43.3% is achieved, attributed to effective suppression of the hydrogen evolution reaction (HER), which is thermodynamically unfavorable above 0 V vs. RHE. The catalyst exhibits high operational stability, retaining 95.5% of current density, due to minimized H₂ bubble formation.

Furthermore, scalability is demonstrated in a zero-gap electrolyzer with a larger active area (3 × 3 cm²), achieving an NH₃ yield of 627 mg h⁻¹ at a current density of 1.5 A cm⁻². These results underscore the strong potential of CoNiCuRu/MWCNT as an efficient and scalable platform for sustainable nitrate-to-ammonia conversion. Future efforts will aim to elucidate the reaction mechanisms to support industrial application.

Keywords: Electrochemical ammonia synthesis, Electrocatalyst, Nitrate reduction reaction, Energy Efficiency, Nitrate remediation



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EFFICIENT SELF-CATALYTIC REACTORS FOR CATALYTIC C1 MOLECULAR CONVERSION

Hao Huang^a, ChengWei Wang^a, YingLuo He^a, Noritatsu Tsubaki^{a*}

^aUniversity of Toyama (Department of Applied Chemistry, School of Engineering, Toyama, Japan).

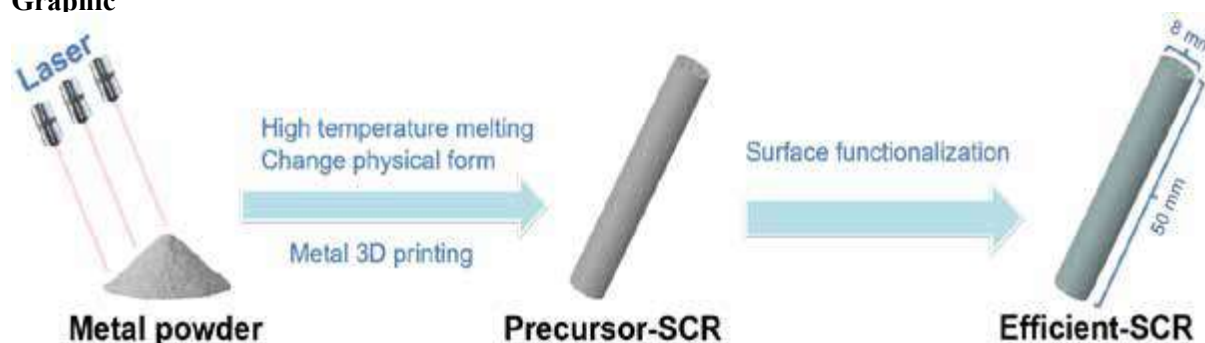
*Corresponding author: tsubaki@eng.u-toyama.ac.jp

Abstract

The depletion of petroleum resources, escalating environmental pollution, and the growing demand for fuels and high-value chemicals have drawn considerable attention to C1 chemistry. The catalytic conversion of one-carbon (C1) molecules such as CO, CO₂, and CH₄ into value-added chemicals and liquid fuels is vital for the chemical industry and aligns with the principles of green chemistry. However, the inherent stability of C-H and C-O bonds, coupled with the uncontrollable formation of C-C bonds, presents significant challenges for selective activation and controlled conversion into high-value products. Additionally, issues related to reaction selectivity, energy efficiency, and emissions remain major hurdles due to the complexity of these processes. Consequently, developing efficient C1 conversion pathways for the targeted production of liquid fuels and high-value chemicals necessitates innovations in both catalyst design and reaction processes. While metal 3D printing has seen widespread application across various industries, its chemical properties and catalytic functions have not been extensively explored. To address this gap, we propose a self-catalytic reactor (SCR) that integrates multiple catalytic functions. By leveraging 3D printing technology, this design enhances the synergy between catalysts and reactors, reduces reactor size and cost, and improves energy efficiency. This approach enables the efficient conversion of C1 molecules, tackling both energy and environmental challenges, and has the potential to revolutionize traditional catalysis and the chemical industry.

Keywords: C1 chemistry, metal 3D printing, synergy

Graphic



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SELECTIVE HYDROGENATION OF CO₂ TO LIGHT OLEFINS USING ALKALI-PROMOTED IRON CATALYSTS

Babar Ali^a, Khalid Alhooshani^{a,b}, Saheed Adewale Ganiyu^{* a,b}

^a*Interdisciplinary Research Center for Refining & Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran, 31261, Saudi Arabia*

^a*Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia*

**Corresponding author: babar.ali@kfupm.edu.sa*

Abstract

The hydrogenation of carbon dioxide (CO₂) into olefins over alkali-promoted iron catalysts offers a sustainable approach for both CO₂ utilization and the production of value-added chemicals. In this study, we investigate the catalytic performance of iron-based catalysts modified with alkali promoters, such as potassium and sodium, in the selective hydrogenation of CO₂ to olefins. Alkali promotion significantly alters the catalyst's electronic properties, enhancing CO₂ activation and optimizing the reaction pathway towards olefin production while suppressing methane formation. The promoted catalysts exhibit improved selectivity towards light olefins, such as C₂-C₃= and -C₄=, which are vital building blocks in the petrochemical industry. The influence of alkali promoters on catalyst basicity and active site distribution is explored, demonstrating a shift in product distribution favoring olefins over paraffins. The effects of reaction conditions, including temperature, pressure, and H₂ to CO₂ ratio, on olefin yield and selectivity are evaluated. Mechanistic insights revealed that alkali modifiers enhance chain growth formation and improve CO₂ adsorption, leading to more efficient carbon-carbon coupling processes. The results demonstrate that alkali-promoted iron catalysts provide a viable approach for CO₂ valorization, contributing to the development of sustainable olefin production and advancing CO₂-based chemical synthesis.

Keywords: CO₂ hydrogenation, Catalyst, olefins, alkali promoters, Iron carbide

MAGNETIC FIELD-ASSISTED CO₂ REDUCTION: MODULATING MAGNETIC MOMENTS AND MOLECULAR BONDING FOR ENHANCED CATALYSIS

Shilin Wei^a

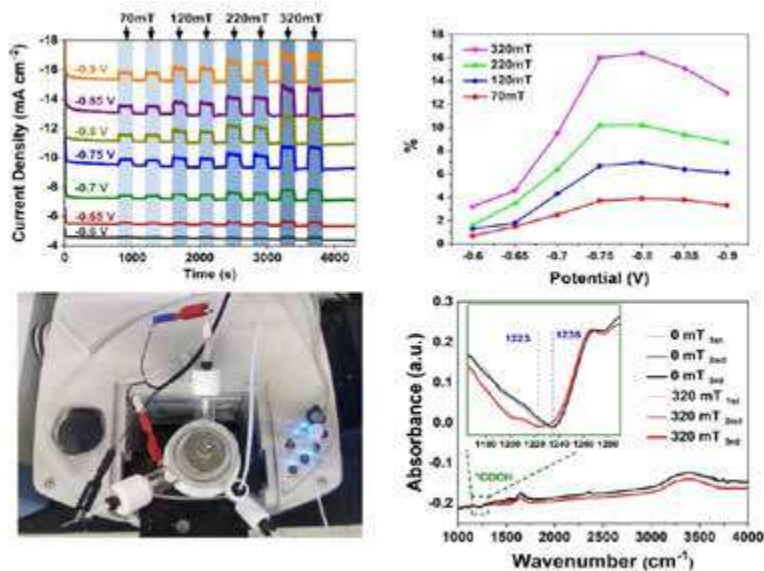
^a*School of Chemical Engineering and Technology, China University of Mining and Technology.*

Corresponding author: shilin.wei@cumt.edu.cn

Abstract

Magnetic fields and electric fields can interact and interconvert. Thus, applying a magnetic field during electrocatalytic processes may exert unique effects on electrocatalysis. This work revealed that the magnetic field could increase the current density in the electrocatalytic CO₂ reduction reaction (eCO₂RR), with higher magnetic field strengths leading to greater current densities. Notably, the enhancement effect of the magnetic field on the current density exhibited a trend of first increasing and then decreasing. This is primarily due to Coulomb repulsion among electrons—higher electron densities at larger potentials result in stronger Coulomb repulsion, which weakens the magnetic field's enhancing effect on the current density. Further electrochemical impedance spectroscopy analysis revealed the underlying mechanism of the magnetic field's enhancement on current density—the magnetic field aligns the magnetic domains of magnetic catalyst, as well as reduces electron scattering and consequently lowers the charge transfer resistance. Additionally, a magnetic gain effect was discovered—the current density at high potentials can be achieved by applying an external magnetic field at low potentials. This magnetic gain effect effectively reduced the energy consumption of the eCO₂RR. On the other hand, the magnetic field also enhanced the Faraday efficiency of CO. To investigate the underlying mechanism, a magnetic-field-equipped operando infrared spectroscopy was designed to capture changes in the molecular structure of the key intermediate *COOH during eCO₂RR. Infrared spectroscopy showed a redshift in the *COOH absorption peak (from 1235 to 1223 cm⁻¹), suggesting that the magnetic field elongated the C–O bond and promotes *COOH dissociation into CO. This finding was further confirmed by density functional theory (DFT) calculations.

Keywords: External field, Magnetic dependence, Molecular level, Multiphysics coupling



ZINC OXIDE NANOSTRUCTURE AND DEFECT MODULATION FOR INTEGRATED ENERGY AND WATER APPLICATIONS

Haw Choon Yian^{*a,b,c,d}, Gan Wee Chen^{a,b,d}, Liow Jo-Ey^{a,b,c,d}, Lim Kok Loong^{a,b,c,d},
Goh Jin He^{a,b,c,d}, Tan Kar Woon^{a,b,c,d}

^aSchool of Energy and Chemical Engineering, Xiamen University Malaysia, 43900 Sepang, Selangor, Malaysia.

^bCollege of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005 China

^cCenter of Excellence for NaNo Energy & Catalysis Technology (CONNECT), Xiamen University Malaysia, Sepang, Selangor Darul Ehsan, 43900 Malaysia

^dKelip-kelip! Center of Excellence for Light Enabling Technologies, School of Energy and Chemical Engineering, Xiamen University Malaysia, Sepang, Selangor Darul Ehsan, 43900 Malaysia

*Corresponding author: cyhaw@xmu.edu.my

Abstract

Zinc oxide (ZnO) nanomaterials have emerged as multifunctional platforms in renewable energy and water purification technologies, where performance can be significantly boosted through structural evolution and defect engineering. This sharing consolidates our recent works from 2022 to present, emphasizing ZnO's role across photothermal solar steam generation (PTSSG), photocatalytic hydrogen evolution, and piezo/triboelectric nanogeneration. In PTSSG, the upcycling of palm fibers into hydrophilic, carbonized scaffolds decorated with ZnO enhanced broadband light absorption, capillary water transport, and thermal localization. Further improvement was achieved via the incorporation of ZnO nanoflowers anchored on 3D palm fiber matrices, delivering superior steam generation and contaminant rejection under low solar flux. In parallel, defect manipulation through controlled gas-phase treatments introduced oxygen vacancies into ZnO crystals, significantly shifting light absorption into the visible range and facilitating photocatalytic hydrogen production under solar irradiation. Complementing these optoelectronic strategies, structural modulation of ZnO arrays—from vertically aligned rods to hierarchical hybrid geometries—yielded a hybrid piezo/triboelectric nanogenerator with enhanced stress transfer, output voltage, and energy harvesting efficiency. Together, these studies underline the synergistic role of nanostructuring and oxygen vacancy engineering in tailoring ZnO's properties, positioning it as a pivotal material for sustainable clean energy, water technologies and low-carbon technological development.

Keywords: Zinc oxide, photothermal, hydrogen evolution, nanogenerator, oxygen vacancies

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BIFUNCTIONAL PHASE-ENGINEERED $\text{NiSe}_2/\text{Ni}_3\text{Se}_4@/\text{NiCoFe-LDH}/\text{NICKEL}$ FOAM NANOSHEETS ELECTROCATALYST FOR EFFICIENT HYDROGEN PRODUCTION AND UREA OXIDATION

Nabilah Saafie^{a, b}, Wee-Jun Ong^{a, b, c, d, e, f, *}

^a School of Energy and Chemical Engineering, Xiamen University Malaysia, Sepang, Selangor Darul Ehsan 43900, Malaysia.

^b Center of Excellence for NaNo Energy & Catalysis Technology (CONNECT), Xiamen University Malaysia, Sepang, Selangor Darul Ehsan 43900, Malaysia.

^c State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China.

^d Gulei Innovation Institute, Xiamen University, Zhangzhou 363200, China.

^e Shenzhen Research Institute of Xiamen University, Shenzhen 518057, China.

^f Department of Chemical and Biological Engineering, College of Engineering, Korea University, 145 Anam-ro, Seongbuk-gu. Seoul, 02841 Republic of Korea.

*Corresponding author: weejun.ong@xmu.edu.my

Abstract

The global energy crisis and environmental pollution have driven the search for sustainable alternatives to fossil fuels. Hydrogen (H_2) is a promising clean energy carrier but conventional production methods are energy intensive and environmentally harmful. Electrocatalytic water splitting offers a green alternative though the oxygen evolution reaction (OER) at the anode remains a bottleneck due to its high overpotential. Urea oxidation reaction (UOR) presents a viable alternative with lower thermodynamic requirements and the added benefit of wastewater remediation. This study aims to develop a high performance bifunctional electrocatalyst for hydrogen evolution reaction (HER) and UOR leveraging phase engineering and heterostructure design to enhance catalytic activity and stability. A self-supported $\text{NiSe}_2/\text{Ni}_3\text{Se}_4@/\text{NiCoFe-LDH}/\text{NF}$ (NSLDH/NF) electrocatalysts was synthesized via a hydrothermal-selenization-electrodeposition approach. The material was characterized using XRD, XPS, SEM, TEM and Raman spectroscopy. The NSLDH/NF catalyst delivered outstanding performance, achieving a remarkably low overpotential of 110 mV to reach 10 mA cm^{-2} for the HER while requiring 1.295 V to drive the same current density for the UOR. Notably, the system exhibited excellent Faradaic efficiencies of 98.90% for HER and 90.97% for UOR, demonstrating its exceptional catalytic selectivity and efficiency. The phase-engineered NSLDH/NF electrocatalyst showcases superior bifunctional activity and practical feasibility for urea-assisted hydrogen production which offers a sustainable pathway for energy conversion and environmental remediation.

Keywords: Bifunctional electrocatalysis, hydrogen evolution reaction (HER), urea oxidation reaction (UOR), layered double hydroxide (LDH), phase engineering

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THE POLAR REGIONS AS SENTINEL REGIONS FOR INVESTIGATING CLIMATE ORGANIC POLLUTANT INTERACTIONS

Roland Kallenborn^{a,*}, Yifan Li^b,

^a*Faculty of Chemistry, Biotechnology and Food Sciences (KBM); Norwegian University of Life Sciences (NMBU), Ås, Norway.*

^b*Dalian Maritime University (DMU), Dalian, Peoples Republic of China*

**Corresponding author: roland.kallenborn@nmbu.no*

Abstract

Dramatic environmental changes are being reported in the Arctic and Antarctic regions at an unprecedented pace. Local populations, communities, as well as marine and terrestrial environments are especially affected due to these climate-related changes in the cryosphere. These changes are expected to have significant consequences for environmental systems and local human populations. The rapid reduction of the Arctic cryosphere (ice-associated systems) is identified as a primary driver of ecological stress (i.e., erosion, atlantification) for delicate Arctic ecosystems, infrastructures, and local societies.

Various indicators illustrate the environmental stress caused by climate changes in the Arctic. These include changes in the foraging behavior of top predators, significant alterations in food webs (such as the invasion of species from temperate regions), and shifts in the seasonal migration patterns of marine species. Additionally, the remobilization of previously stored pollutants, as well as the introduction of new emission sources of Chemicals of Emerging Arctic Concern (CEAC), may contribute to altered bioaccumulation profiles and transformation pathways under Arctic (Polar) conditions. Indigenous peoples of the Arctic are also strongly affected, with traditional hunting routines abandoned due to changing migration patterns of marine mammals. Along the Arctic coastlines, many communities are planning to relocate inland due to extensive erosion problems. Furthermore, hygiene issues and water shortages reduce the living quality in many communities, and the exposure profile for pollutants in Arctic communities is clearly affected.

The declining sea ice and cryosphere present new opportunities for access to fossil resources, mineral mining, and shipping routes. As a result, circum-Arctic nations are looking towards the North for economic opportunities while simultaneously fearing environmental changes. Updated information on the consequences of Arctic climate change on emissions and distribution profiles of selected organic pollutants will be presented. Implications for environmental protection, local communities, and economic opportunities will be highlighted, and the potential for conflicting priorities will be discussed based on case studies.

Keywords: Arctic Pollutants, Climate Change, environment, risk assessment

CONCURRENT APPEARANCE OF LATITUDINAL AND LONGITUDINAL DISTRIBUTIONS AND FRACTIONATIONS OF α - AND β -HCHS IN CHINESE RURAL SURFACE SOIL

Yi-Fan Li^{a,b*}, Shuai Hao^a, Wan-Li Ma^a, Li-Yan Liu^a, Zi-Feng Zhang^a, Wen-Long Li^c, Ning-Zheng Zhu^d, Pu-Fei Yang^a, Hong-Liang Jia^b, Min-Gang Cai^e, Roland Kallenborn^f, Derek CG Muir^g

^a IJRC-PTS, State Key Laboratory of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin 150090, China

^b IJRC-PTS, College of Environmental Science and Engineering, Dalian Maritime University, Dalian, China

^c College of the Environment and Ecology, Xiamen University, Xiamen, China

^d Jiaxing-Tongji Environmental Research Institute, Jiaxing 314051, China

^e State Key Laboratory of Marine Environmental Science, Xiamen University, Xiamen 361102, China

^f Faculty of Chemistry, Biotechnology and Food Science (KBM), Norwegian University of Life Science,

^g School of Environmental Sciences, University of Guelph, Guelph ON N1G 2W1, Canada

*Corresponding author: dr_li_yifan@163.com

Abstract:

The concept of global or latitudinal fractionation of persistent organic pollutants (POPs) was suggested in 1993¹ for the first time. In this study, the distributions and fractionations of two isomers of hexachlorocyclohexane (HCH), α - and β -HCH, were analysed in Chinese rural surface soil using a set of soil samples collected in 2005², 2012³, and 2019⁴ to study the life cycle of the latitudinal fractionation of persistent organic pollutants (POPs). The primary longitudinal and secondary latitudinal distribution of α - and β -HCH and together formed the primary longitudinal and secondary latitudinal fractionations were observed concurrently in the surface soil in these three years. Based on these observations, we identified three stages for the life cycle of latitudinal fractionation for α - and β -HCH. In Stage I, the primary fractionation of the two isomers mainly due to the distance from the source regions begins and intensifies with enrichment of the compounds having lower K_{OA} (octanal-air partition ratio) values and the depletion of the compounds with higher K_{OA} values. In Stage II, the secondary fractionation caused mainly by the air temperature gradient begins and intensifies, keeping the fractionation patterns appearing in the Stage I unchanging. In Stage III, the secondary fractionation pattern is weakened mainly caused by local factors, degradation in particular, until its disappearance. The fractionation patterns appearing in the Stages I and II may change.

Keywords: HCHs, POPs; Primary and secondary fractionations; Global fractionation

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ANTARCTICA'S CHEMICAL VOYAGERS; BUILDING A FRAMEWORK FOR POLICY ADVICE

Susan Bengtson Nash^{a,*}

^a*The Antarctic Monitoring and Assessment Programme (AnMAP), Griffith University, 170 Kessels Road, Nathan, QLD 4111, Australia*

**Corresponding author: s.bengtsonnash@griffith.edu.au*

Abstract

Chemical pollution represents catastrophic threat to Planetary Health. In 2021¹, the United Nations Environment Programme (UNEP) declared pollution as part of a triple planetary crisis, alongside biodiversity loss and climate change². Planetary Boundaries research has found that the safe operating space for novel entities such as chemicals has already been exceeded³. In response to the advanced stage of the threat, the 2022 United Nations Environment Assembly committed to the establishment of an intergovernmental science-policy panel on chemicals, waste and pollution prevention (resolution 5.8). These actions signal a need for a step-change in the way chemical production, regulation, and trade is managed globally. A principal vehicle for the protection of environmental and human health from harmful chemicals, has for the past 21 years since its implementation, been the Stockholm Convention (SC). The SC seeks to reduce and eliminate emissions of identified Persistent Organic Pollutants (POPs) to the environment i.e., chemicals with the evidenced properties of i) persistence, ii) environmental mobility, iii) bioaccumulation potential, and iv) toxicity. The Polar regions of the Earth play a special role in supporting timely regulation of new POP candidates under the SC through the provisioning of chemical monitoring data from high latitude environments⁴. Specifically, if industrial or agricultural chemicals are detected in Polar regions, far from their emission source, this represents robust empirical evidence against both of the chemical criteria of persistence and environmental mobility. In addition, there is the inherent issue of increasing chemical contamination in remote polar regions, and the threat they pose to pressured polar ecosystems. Whilst coordinated chemical monitoring has been underway in the Arctic for over 30 years, data from Antarctica and the Southern Ocean is presently unsuitable for temporal trend analyses. In order to address the need for sufficient, continuous and reliable chemical data from the Antarctic region in support of global chemical policy, the Antarctic Monitoring and Assessment Programme was established in 2023 as a special initiative under the Scientific Committee for Antarctic Research, in partnership with the Arctic Monitoring and Assessment Programme, The United Nations Educational Scientific and Cultural Organization, and Griffith University.

Keywords: Chemical Monitoring, Global Chemical Policy, Persistent Organic Pollutants, Antarctica

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SHIFTS IN PESTICIDE CONTAMINATION IN ARCTIC FJORDS: A PRE- AND POST-COVID ASSESSMENT

Dr Anu Gopinath

*Department of Aquatic Environment Management
Kerala University of Fisheries and Ocean Studies, Kochi, Kerala, India.
Corresponding author: dranugopinath@gmail.com*

Abstract

The distribution and persistence of pesticides in Arctic fjords are influenced by historical inputs, contemporary sources, and environmental transport mechanisms. This study investigates organochlorine pesticides (OCPs) and emerging contaminants in the surface sediments of Kongsfjord and Krossfjord over the timeframes of pre-COVID (2018–2019) and post covid which is the most recent assessment (2023–2024). Pre-COVID data revealed the presence of DDT and its metabolites (p,p'-DDE, p,p'-DDD) alongside emerging pesticides such as diuron, chlorpyrifos, dicofol, pendimethalin, and bifenthrin, with higher concentrations of 0.3355 ng/g (dicloran) in Krossfjord due to localized inputs. Post-COVID analysis indicated shifting contamination patterns, likely influenced by global reductions in industrial and agricultural activities. The most recent data (2023–2024) showed a significant increase in diuron concentrations, while only DDT metabolites persist with a maximum concentration of o,p'- DDT (0.2179 ng/g) highlighting the degradation of parent compounds and ongoing contaminant transport. Higher contamination near open-sea stations suggested transboundary pollution via oceanic and atmospheric pathways. The presence of pesticides in glacial-fed stations indicated possible release from melting ice, emphasizing the role of climate change in remobilizing legacy pollutants. These findings underscore the need for long-term monitoring and international regulatory efforts to mitigate emerging threats to Arctic marine ecosystems.

Keywords: Organochlorine pesticides, diuron, DDT metabolites, glacial melt, transboundary pollution, sediment contamination.

MONITORING OF CONTAMINANTS OF EMERGING CONCERN IN THE SEDIMENTS OF ARCTIC FJORD: ACTIVITIES OF MAHATMA GANDHI UNIVERSITY, INDIA

Nejuma Khalid^a, John Richard Thomas^a, Charuvila T. Aravindakumar^{a,b*}

^aSchool of Environmental Sciences, ^bInternational Centre for Polar Studies,
Mahatma Gandhi University, Kottayam, Kerala, India

*Corresponding author: cta@mgu.ac.in

Abstract

Over the past several decades, the pollution and fate of contaminants in the Polar Regions have become critical areas of investigation. Research groups around the world are actively investigating the presence of chemicals of emerging concern (CECs) in the Arctic environment. Among the various analytical techniques used for their identification and quantification, chromatography coupled with mass spectrometry has proven to be the most effective. Our research group at Mahatma Gandhi University has been participating in the Indian Arctic Expedition for over a decade, contributing to this global effort. In this study, we analyzed sediment samples from Kongsfjorden and Krossfjorden—two sites in the Arctic—using ultra-performance liquid chromatography coupled with high-resolution mass spectrometry (UPLC-Q-ToF-MS). Among the seven selected sampling sites, bisphenol S (BPS), a known plasticizer and CEC, was detected and quantified in three sediment samples from Kongsfjorden at concentrations of approximately 0.2 ppm. Additionally, four major surfactants—decylbenzenesulfonic acid, undecylbenzenesulfonic acid, 2-dodecylbenzenesulfonic acid, and tridecylbenzenesulfonic acid—were identified. A potential BPS metabolite, a sulfur trioxide derivative, was also detected in one sample. The presence of these CECs is likely linked to prolonged human activity in the region. In a subsequent round of sampling, we detected metoprolol, propranolol, lidocaine, and mefenamic acid at microgram-per-liter concentrations, along with eleven additional non-target compounds in the Arctic environment.

Keywords: Chemicals of Emerging Concern, Arctic environment, Mass spectrometry, Non-target analysis, Kongsfjorden and Krossfjorden.

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FINDING ALTERNATIVES TO THE MANY USES OF PFAS

Ian T. Cousins

Department of Environmental Science, Stockholm University, Sweden.

**Corresponding author: ian.cousins@aces.su.se*

Abstract

Globally, the momentum to phase out the “non-essential” uses of per- and polyfluoroalkyl substances (PFAS) is growing based on concerns regarding their high persistence and other hazardous properties that trigger additional concerns. In Europe, such a broad phaseout of PFAS was taken a step towards reality when the national authorities of five European countries submitted a restriction proposal under the REACH Regulation to restrict the manufacture, placing on the market and use of PFAS. Simultaneously, however, there is a recognition among regulators that an outright ban on all PFAS uses is neither practical nor feasible in the short term given their wide use in modern society, including in the green energy transition and healthcare. In a recent study published in the journal *Environmental Science and Technology*, we assessed potential alternatives to PFAS across 325 applications in 18 industries and identified 530 PFAS-free alternatives. While many chemical substitutes were found, the research also highlighted the importance of considering material innovations, process changes, and entirely new technologies. These alternatives can often offer safer, more sustainable solutions than simple chemical substitution. Our study, which was part of the ZeroPM project, employed a functional substitution approach, mapping PFAS according to the functions they fulfil in an application. For 40 applications, potential alternatives to PFAS are already available. However, for 83 applications no suitable alternatives could be identified, underscoring critical research gaps. Furthermore, some identified chemical substitutes raised new concerns, with 31% of the alternatives potentially introducing unforeseen hazards. Our study emphasised the urgent need for collaboration within industry and across sectors, as well as the importance of open data sharing. The ZeroPM alternatives database, available online, aims to centralise knowledge on PFAS-free options, helping regulators and industry leaders make informed decisions.

Keywords: functional substitution, regrettable substitution, alternatives assessment, PFAS-free, database

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HARNESSING MECHANOCHEMISTRY TO SOLVE REAL-WORLD PFAS CHALLENGES

Kapish Gobindlal^{a,b,*}, Marcus Glucina^a, Jonathan Sperry^b

^a*Environmental Decontamination (NZ) Limited.*

^b*University of Auckland.*

**Corresponding author: kapish.gobindlal@edl-tech.com*

Abstract

The global environmental sector urgently requires innovative solutions to address the increasing prevalence of complex PFAS-related challenges (e.g., AFFF stockpiles, highly contaminated soil, spent sorbents). Effectively treating PFAS is a highly regulated and complex facet of the hazardous waste industry that considers efficacy, scalability, cost, and treatment time. PFAS exhibit extreme persistence and physicochemical properties that are resistant to targeted degradation, making effective treatment problematic. Mechanochemical destruction (MCD) is an emerging treatment technology that utilises high speed ball milling to initiate and propagate the mineralisation of PFAS.

In the initial phases of R&D, a comprehensive analytical approach was undertaken to determine the fundamental underlying mechanisms of MCD reactions for PFAS destruction. The overall process was characterised by conventional techniques, such as liquid chromatography-tandem mass spectroscopy, Fourier transform infrared, and surface area analysis. More novel techniques were also employed, including high resolution mass spectrometry, solid-state nuclear magnetic resonance, and electron paramagnetic resonance.

Initial results from laboratory prepared ‘ideal’ samples revealed high destruction efficiencies ranging from 99.95% to 100% for PFAS standards subjected to MCD conditions.¹ Results indicated that the mineralisation of PFAS by MCD occurs via a complex collection of multiple mechanisms operating simultaneously.¹ Based on the intermediates identified as part of the degradation product analysis, core mechanistic steps were developed for the first time.

The MCD technique has recently been applied to ‘real-world’ challenges, specifically for the destruction of PFAS in highly contaminated soil from firefighting training facilities as well as AFFF concentrates. Upon mechanochemical treatment, PFAS were indiscriminately and effectively destroyed. The observed destruction efficiencies ranged from 99.99% and 100% for a wide range of PFAS present in the authentic samples, demonstrating the capability of the MCD technique to address relevant PFAS challenges.² Ongoing work is focused on scaling up MCD for PFAS-laden matrices and PFAS-containing products.

Keywords: PFAS destruction, mechanochemistry, ball milling.

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GROWING EVIDENCE OF HUMAN AND ENVIRONMENTAL EXPOSURE TO PFAS IN ASIA

Rai Kookana^{a*}, Bo Sha^b, Jobriell Baluyot^c, Karl Bowles^d, Melanie Kah^e, Lokesh Padhye^{f,g}, Guang-Guo Ying^h, Divina Navarro^a, Michael Velarde^c, Christopher Higginsⁱ and Ian Cousins^b

^a Commonwealth Scientific and Industrial Research Organization, Environment Research Unit.
The University of Adelaide, Waite Campus, Urrbrae, SA 5064, Australia.

^b Department of Environmental Science, Stockholm University, SE-10691 Stockholm.

^c Institute of Biology, University of the Philippines Diliman, Quezon City, Philippines.

^d Jacobs, 177 Pacific Hwy, North Sydney, NSW 2060, Australia.

^e School of Environment, The University of Auckland, Auckland, New Zealand.

^f The New York State Center for Clean Water Technology, Stony Brook University, NY 11794, USA.

^g Department of Civil and Environmental Engineering, The University of Auckland, New Zealand.

^h South China Normal University, University Town, Guangzhou 510006, China.

ⁱ Colorado School of Mines, Golden, Colorado 80401, USA.

*Corresponding author: kookana@gmail.com

Abstract

The production and use of per- and polyfluoroalkyl substances (PFAS) in certain countries, combined with uncertainties regarding their applications across Asia, highlight the urgent need to assess human exposure—particularly beyond China, Japan, and South Korea, which account for 80–90% of existing environmental PFAS studies.

Exposure levels vary significantly across the region, with industrial activities—such as fluorochemical production, textiles and automotive manufacturing—driving severe PFAS contamination, particularly in freshwater sources. Studies have detected PFAS in surface and groundwaters across 20 Asian countries (~3,000 samples), sometimes at concerning concentrations.

There is now substantial evidence from China, South Korea, and Japan confirming the widespread presence of long-chain PFAS (C₈–C₁₁) in human serum and breast milk. Furthermore, replacement compounds and their degradation products are increasingly being detected in human samples. While data from the rest of Asia remains limited, the extensive contamination of water and food in these countries suggests that human exposure is highly likely too. Beyond direct contamination, additional risk factors may exacerbate exposure in some countries. However, despite growing concerns, PFAS regulations in Asia lag behind those in Western countries, and there is less urgency to characterize exposure levels and associated health risks. The diverse PFAS use and exposure scenarios across Asia underscore the need for broader, more comprehensive research to effectively assess contamination levels, exposure pathways, and potential health risks.

Keywords: Per- and polyfluoroalkyl substances (PFAS); Human exposure; Environmental contamination; PFAS presence in Asia; PFAS occurrence in food and water.

OCCURRENCE OF PFAS IN NEW ZEALAND

Shailja Data^{a,b,*}, Lokesh P. Padhye^c, Melanie Kah^a, Erin M. Leita^{a,b}

^a University of Auckland, New Zealand

^b MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

^c NYS Center for Clean Water Technology, Stony Brook University, USA

*Corresponding author: sdat751@aucklanduni.ac.nz

Abstract

Per- and polyfluoroalkyl substances (PFAS) are a broad class of synthetic fluorinated chemicals. PFAS are widespread in our everyday lives due to their surfactant properties, excellent water and oil repellence and resistance to degradation. However, persistence, bioaccumulation and long-range transport have led to the global detection of PFAS in environmental media.¹ The human exposure to these forever chemicals via ingestion of contaminated food and water, inhalation, dermal contact and occupation exposure has been linked to adverse health effects.² Thus, understanding the extent and exposure of PFAS contamination has garnered increased global attention. While New Zealand (NZ) does not manufacture PFAS, they have been found in the local environment due to their historical use in firefighting foams, importation of consumer products and waste disposal containing PFAS-containing materials, which contribute to PFAS contamination. Though progress has been made in understanding the PFAS burden in NZ's environment, there is still limited knowledge on monitoring studies and exposure pathways. Our project includes a multifaceted approach to understanding the PFAS burden in NZ's environment by filling in knowledge gaps. We first collected the existing PFAS monitoring data in NZ including landfill leachates, wastewater, soil, and biota by compiling existing publicly available reports and requesting data from the regional councils. It was then complemented with missing data by investigating the occurrence of PFAS in drinking water and household dust. Overall, the collated data indicates that studied PFAS levels are relatively lower in NZ compared to other developed nations. However, continuous monitoring is needed for the emerging secondary sources. This presentation will be focused on results from PFAS monitoring studies in NZ in different environmental media with global comparisons. Correlation with housing characteristics and lifestyle factors for PFAS levels in indoor dust will be presented too.

Keywords: Short-chain PFAS, PFAS in environment, PFAS exposure pathways



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MICROBIAL TRANSFORMATION OF PERFLUOROBUTANESULFONIC AND PERFLUOROHEXANESULFONIC ACID

Marija Ljesevic^a, Natalija Petronijevic^b, Branka Loncarevic^a, Caroline Michel^c, Hafida Tris^c, Marc Crampon^c, Fabienne Battaglia-Brunet^c, Latinka Slavkovic Beskoski^d, Vladimir Beskoski^{b,*}

^aUniversity of Belgrade, Institute of Chemistry, Technology and Metallurgy

^bUniversity of Belgrade, Faculty of Chemistry

^cBureau de Recherches Géologiques et Minières, BRGM

^dAnahem laboratory ltd, Belgrade, Serbia

*Corresponding author: vbeskoski@chem.bg.ac.rs

Abstract

Per- and polyfluoroalkyl substances (PFAS) have emerged as significant environmental pollutants due to their persistence and widespread use. Among these, perfluorobutanesulfonic acid (PFBS) and perfluorohexanesulfonic acid (PFHxS) represent shorter-chain alternatives designed to replace longer-chain PFAS such as perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA); however, their persistence and potential ecological impacts are becoming increasingly apparent. PFHxS is third among the PFAS detected in the environment and organisms, followed by PFOS. Additionally, bioaccumulation of PFHxS is higher than that of PFOS and PFOA.^{1,2} Microbial degradation of per- and polyfluorinated alkyl substances (PFAS) is an emerging area of research for mitigating environmental contamination.³ This study explores the microbial degradation potential of PFBS and PFHxS using three different microbial strains isolated from PFAS-contaminated sites. Laboratory-scale degradation experiments were monitored using a Micro-Oxymax Respirometer, which monitors the consumption of O₂ and production of CO₂. Degradation pathways were elucidated by identifying transformation intermediates through liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS). Respirometric results give a good overview of microbial activity in real time and indicated that none of the tested strains were inhibited in the presence of PFBS and PFHxS. One strain exhibited higher activity compared to the others, with the greatest activity observed in the presence of PFHxS.

Keywords: PFBS, PFHxS, microbial degradation, PFAS

Acknowledgement

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UNVEILING THE HIDDEN THREAT OF PFAS CONTAMINATION WITH HIGH-RESOLUTION MASS SPECTROMETRY

Cheah Chris*, Patel Dhaval

Thermo Fisher Scientific, 1 Science Park Road, Singapore Science Park 2, Singapore 117528

*Corresponding author: chris.cheah@thermofisher.com

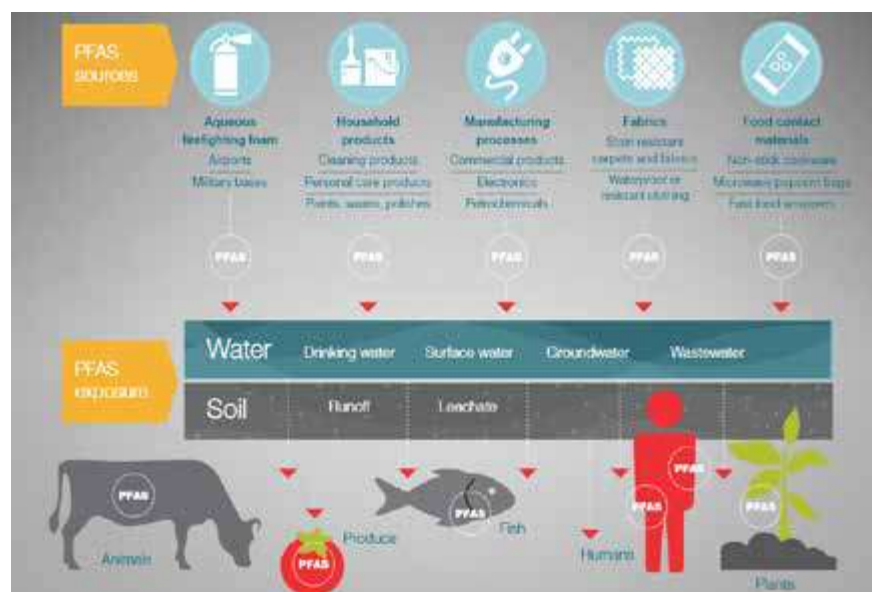
Abstract

Per- and polyfluoroalkyl substances (PFAS) represent a vast and persistent class of environmental contaminants with significant implications for human health and ecological systems. Due to their chemical stability and resistance to degradation, PFAS have become a priority for environmental monitoring and regulatory agencies worldwide. However, the detection and quantification of PFAS at trace levels remain analytically challenging, especially in complex environmental matrices.

The purpose of the presentation is to explore and to illustrate method development strategies for targeted and non-targeted PFAS analysis, including sample preparation approaches, chromatographic separation techniques, and optimized acquisition methods using electrostatic orbital high-resolution mass spectrometry (HRMS). Case studies will demonstrate how HRMS technology enables comprehensive PFAS profiling in various matrices such as drinking water, soil, food and biological samples including workflow to uncover unknown PFAS compounds through suspect screening and data-dependent/independent acquisition, thus expanding the scope of surveillance.

Whether applied in regulatory compliance, environmental risk assessment or research, attendees will gain insights into overcoming analytical hurdles, ensuring data confidence, and ultimately contributing to more effective PFAS monitoring and mitigation strategies.

Keywords: per- and polyfluoroalkyl substances (PFAS), environmental contaminants, untargeted analysis, high-resolution mass spectrometry



RESEARCH ON ENERGY TRANSITION AND SECURITY BASED ON DIGITAL TECHNOLOGY MODEL FOR CHINA

Peng Wang^{a,*}, Hai Tao^a

^a Guangzhou Institute of Energy Conversion, Chinese Academy of Sciences, Guangzhou, Guangdong, 510640, China.

*Corresponding author: wangpeng@ms.giec.ac.cn

Abstract

This study is conducted in the context of unprecedented changes in various dimensions of the climate system, focusing on the energy transition and security in China based on digital technology. The research content encompasses several key aspects. Firstly, it examines national strategies for achieving carbon peaking and carbon neutrality, emphasizing this as a major strategic decision made by the Party Central Committee with Xi Jinping at its core¹. Secondly, it explores the rapid development of renewable energy and its role in energy transition and security. This includes the promotion of green development, the harmonious coexistence of man and nature, and the coordination of industrial structural adjustment in response to climate change. In terms of research methods, the study utilizes a variety of approaches. It involves the investigation of energy-related policies and recommendations provided by government think-tanks^{2,3}. Digital energy technology and low-carbon policies are also analyzed to promote the large-scale application of photovoltaic power generation in the Belt and Road countries^{4,5}. Furthermore, big data platforms for energy economy in Guangdong Province and intelligent energy systems for industrial parks are examined. This study's innovation lies in its comprehensive integration of digital technology with energy transition strategies, emphasizing the use of intelligent systems for renewable energy management. It introduces a detailed roadmap for achieving carbon neutrality by 2060, highlighting the role of photovoltaics and energy storage technologies. The document also outlines a dynamic energy supply-demand warning system and a smart energy monitoring platform, showcasing advanced tools for energy efficiency and economic analysis. These aspects demonstrate a forward-thinking approach to addressing climate change through innovative technology applications. The research concludes that China has set ambitious goals for carbon emissions, striving to peak before 2030 and achieve carbon neutrality by 2060. The development of renewable energy, especially photovoltaic power, has been rapid, with China's photovoltaic industry having a strong competitive edge globally. However, there are challenges such as safety standards missing, inefficient operation and maintenance, and grid consumption issues. Based on the findings, several policy suggestions are proposed. It is recommended to build a dual-carbon technology support system from the perspectives of material flow, energy flow, and value flow. The overall assessment of key technologies should consider technical feasibility, economic viability, and environmental impacts throughout their lifecycle. International cooperation should be strengthened to share experiences and promote the application of innovative technologies and policies abroad. Additionally, comprehensive training on photovoltaic technology and low-carbon policies should be conducted for countries along the Belt and Road. In conclusion, this study provides valuable insights into China's energy transition and security strategies based on digital technology. It highlights the importance of renewable energy development, the challenges faced, and the policy measures needed to achieve sustainable development goals.

Keywords: Energy Transition, Carbon Neutrality, Digital Technology, Photovoltaic Power Generation, Belt and Road Initiative

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CARBON CAPTURE, UTILIZATION AND STORAGE – DEVELOPING COUNTRY PERSPECTIVE

Bipul Behari Saha

Shree Chaitanya Education Society's IGI

drbsaha@rediffmail.com

Abstract

The importance of Carbon Capture, Utilization and Storage is well known. Carbon capture technologies are essential to reduce the carbon footprint. In developed countries, extensive work has been done to develop different technologies for Carbon capture. In spite of some issues, Carbon Capture, Utilization and Storage have been implemented commercially in developed countries.

In developing countries, although some work is going on, there are many challenges in adopting CCUS. Some of these are lack of finance and infrastructure, non-availability of technical expertise, inadequate legal and regulatory framework, constraints on geological sites, economic feasibility and getting international support.

However, some work on CCUS is in progress in India, South Africa, Brazil, Mexico, UAE and other countries. The situation can improve with policy support, financial backing, technology assistance and international cooperation. Details will be discussed.

Keywords: CCUS, Carbon Capture, Developing countries, India

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TORAY GROUP'S GHG REDUCTION INITIATIVES

Tsuneyuki Yamane^{a,*}, Kazuki Goto^b

^aToray Techno Co., Ltd.

^bToray Industries, Inc.

*Corresponding author: tsuneyuki.yamane.z6@ttk.toray

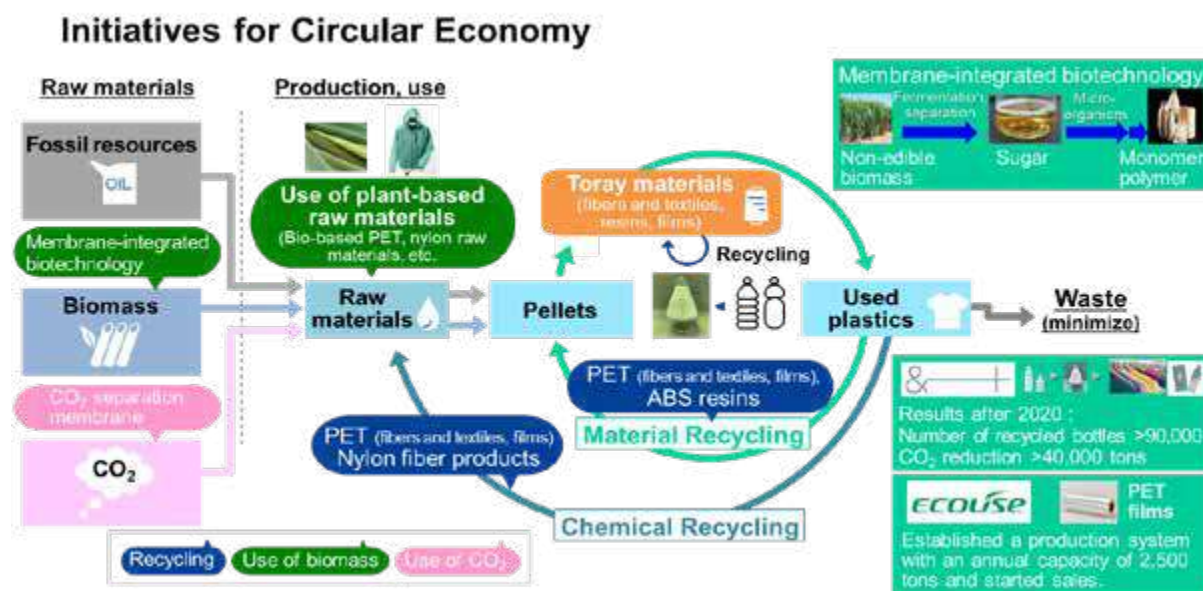
Abstract

At the TORAY Group, we consider sustainability to be the most important global issue of the 21st century. Since TORAY's founding in 1926, we have always believed that "materials can change lives". We make it our mission to deliver innovative technologies and advanced materials that provide real solutions to the challenges the world faces with balancing development and sustainability. By delivering on our corporate philosophy of "contributing to society through the creation of new value with innovative ideas, technologies and products," we will do our utmost to address global issues, while working closely with our business partners worldwide.

After introduction of TORAY Group Sustainability Vision, our activities for Scope 3 achieving circular economy society, namely our activities for "how to make raw materials carbon neutral" will be presented.

1. As a material company, TORAY's first approach is to promote material recycling. TORAY has already started this approach for polyester fiber & textile, PET film, and ABS & PPS resins.
2. The second approach is chemical recycling. From a CFP perspective, we believe that chemical recycling of polymer to monomer rather than to naphtha is more desirable. In this approach, we will present our current development activities for chemical recycling system for nylon & PET.
3. In order to respond to growing demand, we are developing biomass-based materials from non-edible biomass, and also developing CO₂ based chemicals as a Third approach.

Keywords: Material & Chemical recycling, Non-edible biomass, Plant-based chemicals, Membrane-integrated biotechnology



HARMONIZING REPORTING STANDARDS AND EVALUATING ADVANCED CARBON CAPTURE TECHNOLOGIES

Diane Purchase^{a,*}, Michelle Bailey^b, Weiping Wu^c,

^a*Faculty of Science and Technology, Middlesex University, London, UK.*

^b*National Institute of Standards and Technology, Gaithersburg, USA.*

^c*Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai, China.*

*Corresponding author: d.purchase@mdx.ac.uk

Abstract

The evaluation of Carbon Capture, Utilization, and Storage (CCUS) technologies is a critical for achieving global climate targets. However, the diversity of technologies and methodologies across terrestrial, aquatic, and atmospheric compartments presents challenges in standardisation¹, scalability², economic prospects³ and effectiveness⁴. Two IUPAC projects aim to address these challenges through 1) harmonizing reporting requirements for carbon accounting platforms and 2) developing a framework for assessing advanced CCUS technologies.

To evaluate reporting requirements, a survey is in progress of major accounting platforms used across the globe. We aim to understand each platform's requirements for assessing additionality, causality, permanence, and risk management alongside accepted measurement approaches and measurement uncertainty for terrestrial carbon projects. After the assessment is complete, we will produce a report that highlights similarities, differences, and recommendations for standardized practices.

The second project is developing an assessment framework which will focus on five major areas that are essential for ensuring the effectiveness and long-term viability of CCUS solutions: Technological and Operational Performance, Economic and Market Viability, Environmental and Sustainability Considerations, Safety, Compliance and Social Impact, and Transparency, Innovation, and Risk Management.

The scoring system applies a quantitative 1–5 scale to each criterion, incorporating compliance with established carbon accounting platforms, also being evaluated for reporting requirements, such as the Verified Carbon Standard (VCS), Gold Standard, and Greenhouse Gas (GHG) Protocol. The framework offers a structured and standardised approach for evaluating CCUS technologies, enhancing comparability and fostering best practices across sectors and supports the development of scalable, cost-effective, and environmentally sustainable carbon management solutions, accelerating progress toward net-zero emissions.

Keywords: Carbon Capture Utilization and Storage (CCUS), Standardized Assessment Framework, Technological Performance, Environmental Sustainability, Climate Change Mitigation

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THE ENGINEERED PLATFORM FOR BIO-ETHYLENE PRODUCTION FROM ATMOSPHERIC RESOURCE, CO₂

Sadanari Jindou^a, Hiroto Tamura^{b,*}

^a Faculty of Science and Technology, Meijo University, Nagoya, Aichi 468-8502 Japan

^b Department of Environmental Bioscience, Meijo University, Nagoya, Aichi 468-8502 Japan

*Corresponding author: hiroto@meijo-u.ac.jp

Abstract

Ethylene, one of the important industrial raw materials, is made by high-temperature cracking of naphtha, generating 3 t of CO₂ into the atmosphere. Therefore, based on the synthetic biology, we have developed an ethylene-producing strain of the cyanobacterium *Synechococcus elongatus* PCC7942, which platform utilizes 3 t of atmospheric CO₂ per 1 kg ethylene. This genetically engineered cyanobacteria, *S. elongatus* PCC7942 had a unique synthetic life form that consists of three functions. The first was achieved by introducing the 1-amino-cyclopropane-1-carboxylic acid (ACC) synthase (ACS) and ACC oxidase (ACO) from tomato (*Solanum lycopersicum*), which are plant-derived enzymes involved in ethylene biosynthesis. In addition, these two enzymes were converted to chimeric enzyme complex (SOC2) using the cohesin-dockerin interaction from two cellulolytic anaerobic bacteria, *Clostridium thermocellum* and *Acetivibrio cellulolyticus*. Therefore, two ethylene-forming enzymes, ACS and ACO, can be placed in tandem to produce bioethylene with an efficiency of 0.17 mg/L•day. This bioethylene synthesis activity was increased 3.7-fold by chimeric enzyme complex formation rather than free enzymes, suggesting that this chimeric complex of two enzymes was constructed by designer cellulosome concept to enhance the substrate channeling of their two catalytic reactions for ethylene synthesis. Moreover, when the ribosome binding site was optimized for cyanobacteria, the ethylene production activity of SOC2-RBS34 strain increased approximately two-fold. The current production level remains at a micro-scale production compared to the production scale required for commercialization. However, our platform can increase the number of enzymes as we want by using the cohesin-dockerin interaction system. In progress, to increase production efficiency of bioethylene, novel chimeric enzyme complex, named SOC6 strain, was designed to accumulate four ACOs. In summary, the development of a bioethylene production platform using engineered cyanobacteria represents a game-changing advance in sustainable industrial biotechnology. The platform we have established can produce useful substances using atmospheric carbon dioxide as a resource.

Keywords: Ethylene, Cyanobacteria, *Synechococcus elongatus*, cellulosome, dockerin, cohesin

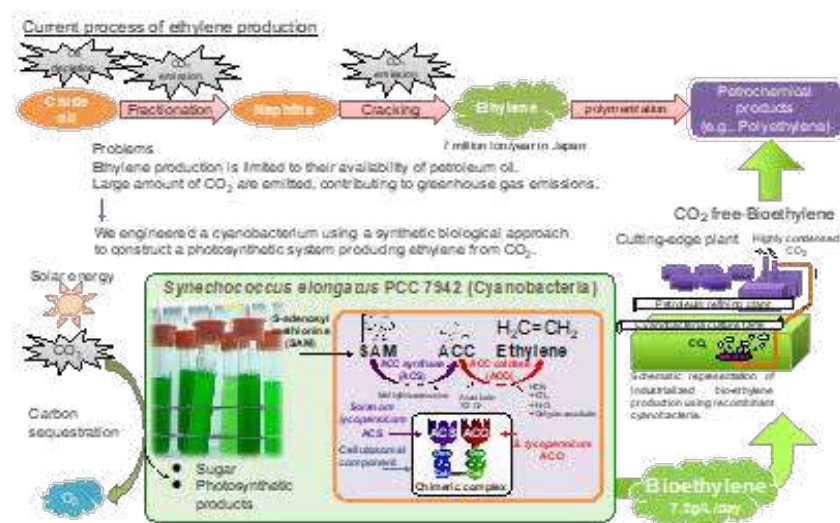


Figure Bioethylene production from CO₂ by an engineered cyanobacteria

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DOW AMINES: FROM PRODUCTION TO CO₂ CAPTURE APPLICATIONS

Xue (Ida) Chen^{a*}

^a*The Dow Chemical Company, Lake Jackson, TX, USA*

**Corresponding author: chen2c7ab2@dow.com*

Abstract

Solvent-based absorption methods are among the most recognized and widely used techniques at a commercial scale for CO₂ capture across various sectors, including power and heat generation, natural gas sweetening, and hydrogen production. Dow's amine products, as a key component of solvent-based absorption technology, play a significant role in CO₂ capture applications. Over the past decades, Dow's R&D team has developed advanced catalysts and processes to enhance the production of these amines. This presentation will detail the journey from laboratory research to pilot projects and full-scale plant operations, showcasing the evolution and impact of these advancements. Additionally, the presentation will cover the characteristics and structures of various amines, highlighting their respective advantages and disadvantages. This comprehensive overview will provide insights into the selection and application of amines for different CO₂ capture scenarios. To further enhance efficiency and reduce the overall cost of these processes, new amine molecules are being developed. These developments focus on improving CO₂ absorption capacity, optimizing application in equipment, and reducing solvent regeneration energy. By advancing the performance and cost-effectiveness of amine-based CO₂ capture, Dow continues to lead the way in sustainable and innovative solutions for carbon management.

Keywords: amines, carbon capture, decarbonization

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TUNING UiO-66-SO₃H FOR SUPERIOR CO₂ ADSORPTION WITH DUAL LIGANDS

Lee Peng Teh^{a,*}, Siva Rubini Devi Raveendran^a, Rizafizah Othaman^{a,b}, Chin Hua Chia^c

^a Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia

^b Polymer Research Center, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia

^c Department of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia

*Corresponding author: lpteh@ukm.edu.my

Abstract

Metal-organic frameworks (MOFs) have emerged as promising materials for gas adsorption due to their tunable structures and high surface areas. This study aims to enhance the CO₂ adsorption performance of sulfonated UiO-66 by incorporating a second linker, 2-amino terephthalic acid, using a mixed-ligand strategy. The objectives were to investigate the structural, morphological, and adsorption properties of the modified UiO-66-SO₃H and evaluate its stability and recyclability. X-ray diffraction (XRD) revealed a transition from an amorphous to a crystalline structure, while Fourier transform infrared (FTIR) spectroscopy identified new peaks corresponding to N-H and C-N stretching with the incorporation of second linker. Thermal analysis showed that all modified UiO-66-SO₃H-NH₂ samples retained stability comparable to pristine UiO-66-SO₃H. Field emission scanning electron microscopy (FESEM) indicated a morphological transformation from a round-like shape (UiO-66-SO₃H) to a triangular-based pyramid (UiO-66-SO₃H-NH₂-0.85). Nitrogen physisorption analysis demonstrated a remarkable increase in BET surface area, rising from 16 m²/g (UiO-66-SO₃H) to 706 m²/g (UiO-66-SO₃H-NH₂-0.85). CO₂ temperature-programmed desorption (CO₂-TPD) confirmed the formation of additional medium basic sites due to increased incorporation of second linker. As a result, UiO-66-SO₃H-NH₂-0.85 exhibited a CO₂ adsorption capacity of 2.17 mmol/g, a fivefold improvement over UiO-66-SO₃H (0.43 mmol/g). Both samples demonstrated excellent recyclability, preserving their crystallinity, functional groups, and thermal stability over ten cycles. Stability tests in water and acidic environments confirmed that both UiO-66-SO₃H and UiO-66-SO₃H-NH₂-0.85 retained their original structural integrity, a high BET surface area, and good CO₂ adsorption performance, highlighting their potential for practical CO₂ capture applications.

Keywords: sulfonated UiO-66, mixed-ligand strategy, UiO-66-SO₃H-NH₂-0.85, CO₂ adsorption

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REDUCED GRAPHENE OXIDE AS AN ADVANCED SUPPORT FOR NICKEL CATALYST IN CO₂ METHANATION

Nur Diyan Mohd Ridzuan^{a,b,*}, Maizatul Shima Shaharun^{a,b}

^a*Department of Fundamental and Applied Sciences, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia.*

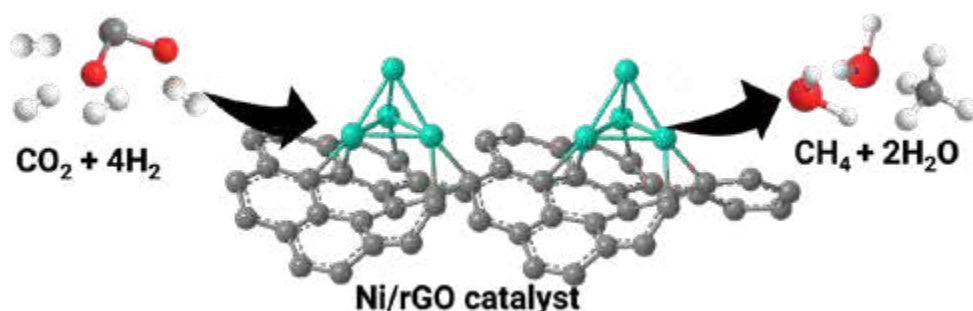
^b*Center of Carbon Capture, Utilization and Storage, Institute of Sustainable Energy, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia.*

**Corresponding author: diyanridzuan@gmail.com*

Abstract

Reduced graphene oxide (rGO)'s high surface area, thermostability, presence of residual oxygen functional group, and exceptional mechanical strength make it a promising material in heterogeneous catalysis, particularly as a catalyst support. In this study, rGO was synthesized *via* chemical reduction method and employed as a support for Ni catalyst *via* impregnation method to produce Ni/rGO. Then, Ni/rGO catalyst are tested for CO₂ methanation at 350 °C, 1 bar, and 4 H₂/CO₂ ratio in comparison to unsupported NiO particles and conventional Ni/Al₂O₃ catalyst to evaluate its efficiency in enhancing CO₂ conversion and CH₄ selectivity. Performance evaluations demonstrated that Ni/rGO (CO₂ conversion of 60.61%) significantly outperformed unsupported NiO (35.32%), attributed to rGO's role in enhancing Ni dispersion, increasing active site availability, and mitigating particle agglomeration, as confirmed by extensive characterization. Compared to NiO nanoparticles, Ni/rGO exhibited a higher surface area (100.01 m²g⁻¹), smaller Ni particle size (6.88 nm), improved reducibility, greater CO₂ adsorption capacity (2.42 mmol g_{cat}⁻¹), and establishment of metal-support interactions. Furthermore, comparative analysis revealed that Ni/rGO also outperformed the conventional Ni/Al₂O₃ catalyst, emphasizing rGO's superior catalytic support properties. Ni/rGO achieved a higher CO₂ conversion (60.61%) than Ni/Al₂O₃ (55.68%), highlighting its effectiveness for CO₂ methanation. The lower performance of Ni/Al₂O₃ is possibly correlated to catalyst poisoning and sintering in the presence of water during reaction. Additionally, Ni/rGO demonstrated an impressive CH₄ selectivity of 99.81% compared to 97.44% for Ni/Al₂O₃, which suggest high ability of Ni/rGO to suppress the formation of CO byproduct from reverse-water-gas-shift reaction. These findings underscore the pivotal role of rGO as an advanced catalyst support for efficient CO₂ methanation. The enhanced performance of Ni/rGO makes it a highly promising candidate for CO₂ methanation integration into power-to-gas technology, facilitating renewable energy storage and contributing to carbon-neutral energy solutions.

Keywords: Reduced graphene oxide; Carbon dioxide methanation; Ni catalyst.



CO₂ HYDROGENATION TO OLEFINS OVER Fe-BASED COMPOSITE CATALYSTS

Zixu Yang^{a,*}, Weifeng Yu^a, Bo Sun^a, Yifan Han^{a,b}

^aEast China University of Science and Technology

^bZhengzhou University

*Corresponding author: zixu.yang@ecust.edu.cn

Abstract

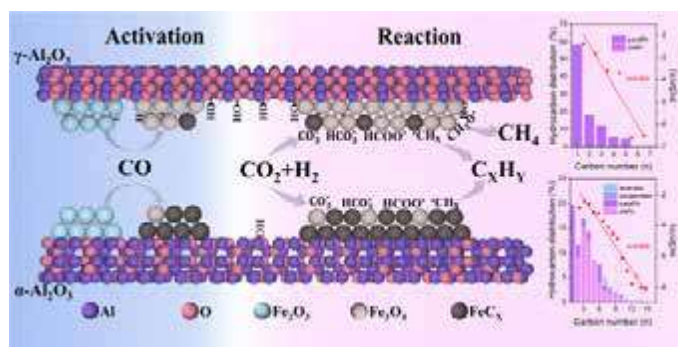
CO₂ hydrogenation offers a promising route for chemical valorization of greenhouse gases, enabling the production of light olefins—key building blocks in the petrochemical industry—via sustainable processes. Among various catalytic systems, Fe-based catalysts are particularly attractive due to their earth-abundance, tolerance to CO₂, and dual functionality: promoting the reverse water–gas shift (RWGS) and Fischer–Tropsch synthesis (FTS) reactions. However, achieving high olefin selectivity remains challenging due to complex reaction pathways and dynamic evolution of the active phases. Recent studies suggest that the structural transformation of Fe species (e.g., Fe, Fe₃O₄, FeC_x) under CO₂ hydrogenation conditions plays a decisive role in catalytic performance. Understanding and controlling this dynamic behavior is therefore crucial for the rational design of efficient catalysts. In this study, we explore Fe-based composite catalysts with tailored architectures, aiming to enhance olefin selectivity and catalyst stability. Key aspects include:

- Bifunctional metal–zeolite systems:** A physically mixed FeZnNa and Na-SAPO-34 catalyst delivered high olefin yield (18.87 mmol·g⁻¹·h⁻¹), enabled by CO spillover and acid site regulation.
- Support phase engineering:** Among γ-, δ-, θ-, and α-Al₂O₃, the α-phase supported Fe catalyst exhibited superior activity and stability, attributed to favorable metal–support interactions and FeC_x generation.
- In situ characterizations:** Techniques such as XRD, FTIR, and Raman were used to track the evolution of active phases and correlate structure with product distribution.

This work highlights the importance of understanding catalyst dynamics as a foundation for designing next-generation Fe-based systems for CO₂ hydrogenation.

Keywords: CO₂ hydrogenation, Fischer-Tropsch synthesis, Olefins, Reaction mechanism, Operando Characterization

Graphic / Image (Optional)



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MEMBRANES FUNCTIONALIZATION WITH NON-VOLATILE SOLVENTS FOR GAS SEPARATION – DES AND ILS AS A SUSTAINABLE APPROACH

Beatriz F. Esteves^a, Bruna R. M. Ferreira^a, Isabella Souza^a, João Peres Ribeiro^a, Filipe H. B. Sosa^a and Pedro J. Carvalho^{a,*},

^aCICECO – Aveiro Institute of Materials, Chemistry Department, University of Aveiro, Portugal.

*Corresponding author: Carvalho.p@ua.pt

Abstract

Over recent decades, greenhouse gas (GHG) emissions have risen, leading to an increase in their atmospheric concentrations and amplifying the natural greenhouse effect. This has resulted in adverse impacts on Earth's ecosystems and climate. The annual GHG emissions are approximately 50 billion tons of CO₂ equivalents, comprising 73.7% carbon dioxide (CO₂), 18.9% methane (CH₄), 4.7% nitrous oxide (N₂O), and 2.7% fluorinated gases.[1] Various technologies, including absorption, adsorption, and electrochemical reduction, have been employed to mitigate these pollutants. However, traditional abatement technologies face several drawbacks, including high energy demand, low efficacy, solvent toxicity and size requirements.[2] These limitations underscore the need for more efficient and environmentally friendly GHG mitigation approaches. Non-volatile solvents, particularly Ionic Liquids (ILs) and Deep Eutectic Solvents (DES) have emerged as promising alternatives to conventional solvents, due to their attractive properties, including negligible vapor pressure, high thermal stability, and tunable properties.[3] However, the direct implementation of non-volatile solvents in conventional separation units faces obstacles, including the need for large separation units and high energy demands for solvent recovery.[4] To address these challenges, we proposed the development of functionalized polymeric membranes based on Pebax®, incorporating non-volatile solvents. This novel approach aims to optimize the balance between the sorption capacity and selectivity of the solvent with the modularity, compactness, and scalability inherent in membrane technology.

Keywords: Deep Eutectic Solvents, Ionic Liquids, Mixed-Matrix Membranes and Gas Separation.

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ADSORPTION ISOTHERM FOR CO₂ CAPTURE USING MANGANESE OXIDE SYNTHESIZED VIA PRECIPITATION METHOD: THE EFFECT OF ADSORBENT ACTIVATION

Muhammad Azli Yusof Nor Azman^a, Azizul Hakim Lahuri^{b,*}, Syawal Mohd Yusof^c, Siti Sarahah Sulhadi^d, Salma Samidin^e, Nur Farhana Jaafar^f, Norazzizi Nordin^g, Norliza Dzakaria^h

^{a,b,c,d}*Department of Science and Technology, Universiti Putra Malaysia Bintulu Campus, Nyabau Road, P.O. Box 396, 97008 Bintulu, Sarawak, Malaysia.*

^e*Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.*

^{f,g}*School of Chemical Sciences, Universiti Sains Malaysia, 11800 USM Pulau Pinang, Malaysia.*

^h*School of Chemistry and Environment, Faculty of Applied Sciences, Universiti Teknologi MARA, Cawangan Negeri Sembilan, Kampus Kuala Pilah, 72000, Kuala Pilah, Negeri Sembilan, Malaysia.*

**Corresponding author: azizulhakim@upm.edu.my*

Abstract

The potential of manganese oxide in various catalysis application related to reaction with CO₂ molecule widely reported. The capability of the MnO in CO₂ capture via adsorption could facilitate in the understanding the CO₂ affinity of the material. A most fundamental reaction of MnO with CO₂ molecule via CO₂ capture was investigated to provide insights of adsorption capacity, desorption temperature and the behaviour of the adsorption process through adsorption isotherm models. The MnO was synthesized using conventional precipitation method with the polyethylene glycol as the surfactant to prevent agglomeration of the particles. The polyethylene glycol and KMnO₄ precursors were dissolved in 1:1 mass ratio with the pH of the solution controlled at pH 7, 8 and 9. After stirring at room temperature, it was rinsed with distilled water and was dried in an oven. The adsorbents were divided to two portions for calcination under ambient air and thermal treatment under N₂ atmosphere at 600 °C. The CO₂ capture study was conducted using CO₂ adsorption isotherm at 25 °C and temperature programmed desorption using CO₂ to measure the adsorption capacity via physisorption and chemisorption, respectively. The MnO-N series adsorbents thermal treated under N₂ shows uniform composition with the presence of MnO alone compared to those calcined under air (MnO-A) contains MnO, Mn₂O₃ and MnO₂. The uniform composition of MnO due to the absence of oxygen and limits oxidation of Mn. The MnO-N9 exhibited the most efficient adsorbent with the highest adsorption capacity due to the most contribution at the medium basic site at around 300-400 °C. The adsorption process reveals that the experimental data best fit with the Freundlich adsorption isotherm model. It implies the CO₂ adsorption occur via multilayer adsorption on heterogeneity surfaces. These results are useful for predicting the appropriate desorption temperature for recyclability test in the future work.

Keywords: Activation method, adsorption isotherm, CO₂ capture, manganese oxide, precipitation method

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RADIOACTIVITY IN THE MARINE ENVIRONMENT: CONTEXT, PERCEPTIONS, AND RISKS

Nicholas D. Priest

Université Laval, Québec, Canada, and Middlesex University, UK.

**Corresponding author: prof.nick.priest@gmail.com*

Abstract

Seventy-one percent of the earth's surface is covered by oceans and seas and changes in the marine environment provide a potential threat to the wider global environment, and human health. Human activities that have produced both local and global impacts are many. In a major recent publication on human health and ocean pollution (Landrigan et al.) pollutants of concern are identified, including plastic waste, spilt oil, chemicals, nutrients, mercury, and pesticides. Radionuclides are not mentioned. In contrast, there is much evidence to suggest that the discharge of radionuclides and exposures to anthropogenic radiation sources generally are of major concern to populations across the world. Radionuclides of most concern are hydrogen-3 (tritium) – as evidenced by concerns about discharges to the Pacific Ocean from Fukushima –, the fission products e.g., caesium-137 and strontium-90, and discharged nuclear fuel radionuclides including uranium and plutonium isotopes. While accidental losses and the sea dumping of fuel cycle wastes are important it is fuel recycling operations that, historically, have resulted in the largest discharges and the greatest accumulations of radioactivity in regional waters and marine sediments. Of these, the operations at the Windscale/Sellafield site in the UK have resulted in the highest regional accumulations of fuel cycle radionuclides – in the Irish Sea. These discharges, most of which occurred in the 1970's, were permitted provided the consequent radiation doses received by the most exposed populations (the critical group) did not exceed the population dose limit for exposures to anthropogenic radiation. In the early years this was set at 5mSv/y and the reference critical group were people that collected and consumed larva bread (contaminated seaweed). At this dose level, and at this time, it was assumed that either the exposures would result in no ill-effects or were too small to be of concern. Subsequently, radiation protection assumptions were changed such that all exposures to radiation were deemed to be carcinogenic and potentially harmful. The level of harm equivalent to 5mSv/y could then be calculated to be approximately 0.025% - although local concerned populations perceive risks to be underestimated. However, when radiation risk factors were specified, they were calculated from the backward extrapolation of high dose toxicity data and may not be relevant to low dose exposures. Moreover, the effects of induced damage repair and immune responses were not fully considered, and recent evidence suggests high environmental exposures in regions of high natural radioactivity have not resulted in the predicted adverse outcomes on health. Moreover, there is new evidence that suggests that low exposures, up to about 100mSv, may actually inhibit the progression of cancer and result in life-extensions. Given that the radiation doses from the marine environment are now much lower than 5mSv/y, it is concluded that there is no evidence to suggest that populations should be concerned about health effects resulting from the contamination of global and local marine environments by radionuclides.

Keyword: Marine, Contamination, Radionuclides, Dose, Hazard

ARTIFICIAL RADIONUCLIDES IN MARINE SEDIMENT

Sakellariadou F

Dept of Maritime Studies, University of Piraeus, Piraeus, Greece.

**Corresponding author: fsakelar@unipi.gr*

Abstract

Anthropogenic radioactive materials enter the marine environment through radioactive fallout from atmospheric nuclear weapons testing, nuclear power plant accidents, radioactive waste dumping, nearshore nuclear facilities discharges, and nuclear ship accidents¹. Also, some of the radionuclides that have been deposited in the terrestrial environment are transported into the sea by river runoff and groundwater discharges¹.

When radionuclides attach to particles in seawater, they sink to the bottom. They return to the water column because of their resuspension. Long-lived radionuclides are buried in subsurface sediments. Radionuclide mobility and bioavailability in soils rely on a soil clay size fraction, clay mineralogy, organic matter, cation exchange capacity, pH, and amounts of competing cations.

The Fukushima Daiichi Nuclear Power Plant accident released numerous anthropogenic radionuclides mostly through atmospheric fallout and to a lesser amount through directed discharges, river runoff and submarine groundwater discharges². They have been transported within the Pacific Ocean. Nearshore sediments off Japan will remain a significant long-term source of radio cesium for years to decades. Artificial radionuclides in the Baltic Sea sediments are greatly impacted by the Chernobyl Nuclear Power Plant accident³. Fallout had an abundance of ¹³⁷Cs and ¹³⁴Cs. There are still remnants in the marine sediments of numerous European countries. In the NE Irish Sea, the main source of ¹³⁷Cs, ²⁴¹Am, ^{239,240}Pu is the nuclear fuel reprocessing facilities at the Sellafield Works of British Nuclear Fuels Ltd. Significant amounts of ¹³⁴Cs, ⁹⁰Sr and ⁹⁹Tc as well as detectable amounts of plutonium and americium have been transported to the Arctic⁴.

In the Mediterranean Sea, most of the radionuclides found are fission and activation products, such as ¹³⁷Cs, ⁹⁰Sr, ^{238,239,240}Pu and small amounts of ²⁴¹Am. A substantial amount of ¹³⁷Cs was added due to the Chernobyl accident¹. The Rhône River transports radionuclides. Fallout from nuclear testing is the main source of Pu. Exchanges across the Gibraltar and the Turkish Straits are other sources.

Keywords: artificial radionuclide, Chernobyl NP accident, Fukushima Daiichi NP accident, marine sediment, Mediterranean Sea

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MEASUREMENT OF URANIUM SERIES RADIONUCLIDES IN SHU RIVER WATERS

Burkitbayev M.M.^{a,*}, Matveyeva I.V.^a

^a*al-Farabi Kazakh National university, Almaty, Kazakhstan*

**Corresponding author: Mukhambetkali.Burkitbayev@kaznu.edu.kz*

Abstract

Shu-Sarysu uranium province is one of the main source of uranium in Kazakhstan. As the Shu river is transboundary river the presented study has international significance.

pH value of the river Shu is in the range $7.74 \div 8.43$, thus water of river Shu are weakly alkaline. The concentration of dissolved oxygen in water samples taken from the river Shu is $7.22 \div 10.4 \text{ mg L}^{-1}$.

The results of determined of uranium isotopes, polonium-210 and lead-210, showed the concentrations less than normative levels. The total concentration of uranium along the river increased in 4.1 times. In the investigated water from Tasotkel dam impoundment and downstream the concentration of total uranium exceeds the normative level (from 15.56 to 39.52 $\mu\text{g L}^{-1}$). This may be due to thinning in Tasotkel dam impoundment of groundwater enriched by uranium up to hazard levels ($10^{-4} - 10^{-5} \text{ g L}^{-1}$) associated with the local uranium anomaly. The concentration of uranium in water from the well of the village Kenes is $83.99 \pm 3.88 \mu\text{g L}^{-1}$, that means 5.6 times higher than the normative level.

To establish the man-made impact the best way is to use the non-equilibrium isotope method. In the studied samples of water is an excess of the daughter product (uranium-234), but the excess is insignificant and indicates the human impact on these waters, including, the source of drinking water in Kenes village (sampling point Ken). Downstream of river Shu, the $^{234}\text{U}/^{238}\text{U}$ isotope ratio decreases, which indicates increase of anthropogenic impact on these waters [1].

The calculation of chemical species of uranium in water showed that in all studied samples uranium is preferably in three forms: $[\text{UO}_2\text{OH}]^+$, $[\text{UO}_2(\text{CO}_3)_2(\text{H}_2\text{O})_2]^{2-}$ and $[\text{UO}_2(\text{CO}_3)_3]^{4-}$. However, despite the significant concentration of sulfate-ions in the water, the probability of detection of sulfate complexes in the analysed water is very low [2].

Keywords: radionuclides, uranium, waters, alpha-spectrometry

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RADIOACTIVITY IN THE IRISH COASTAL ENVIRONMENT: A REVIEW OF 40 YEARS OF INVESTIGATIONS

L. León Vintro^{a,*}, C. Keary^b, J. Murphy^b, L. Morrison^c, A. Collins^{b,d}, O. Hanley^d

^a*School of Physics, University College Dublin, Dublin 4, Ireland.*

^b*School of Science and Computing, South East Technological University, Waterford, Ireland.*

^c*Earth and Life Sciences, School of Natural Sciences, University of Galway, Galway, Ireland.*

^d*Office of Radiation Protection and Environmental Monitoring, Environmental Protection Agency, Clonskeagh Square, Dublin 14, Ireland.*

**Corresponding author: luis.leon@ucd.ie*

Abstract

The Irish Sea contains elevated levels of anthropogenic radionuclides, mainly arising from controlled low-level liquid discharges associated to nuclear fuel reprocessing operations at Sellafield (UK) over the past seven decades. Although taking place over a much longer time span, Sellafield-derived releases for some radiologically important radionuclides (e.g., ¹³⁷Cs, ^{239,240}Pu, ²⁴¹Am) are similar or even larger in scale than the corresponding estimated radionuclide inputs to the ocean following the Chernobyl and Fukushima disasters and have, therefore, been the subject of intense monitoring and research by countries which, like Ireland, have been directly impacted by these releases. In this review, the temporal and spatial evolution of selected artificial radionuclides in key environmental compartments (seawater, sediment, biota) of the Irish Sea are discussed, with emphasis on the chemical and physical processes responsible for their dispersion, accumulation and redistribution, and on the impact of historic and recent discharges to the Irish coastal environment. For most of the nuclides considered, discharges peaked in the mid-to late-1970s, but declined by at least two orders of magnitude by the early-1990s with the introduction of more efficient treatment plants. Although measured radionuclide concentrations in the Irish coastal environment over the past few decades reflect this marked decrease in discharges, the level of reduction observed does not match that of the discharges, highlighting the role played by previously contaminated sediments (now acting as a diffuse source of radionuclides) in controlling the evolution of measured levels, and the importance of solid speciation in determining the rate of remobilisation from sediment into the water column. Although concentrations of artificial radionuclides along the north-eastern Irish coast remain significantly higher than those found in adjacent marine areas, past and present radionuclide levels are of little radiological significance, particularly when compared to the doses associated with similar pathways of exposure from natural sources.

Keywords: Irish Sea, Sellafield, radiocaesium, plutonium, remobilisation

^{137}Cs DISPERSION IN COASTAL OCEAN FOLLOWING THE FUKUSHIMA DAIICHI NUCLEAR POWER PLANT ACCIDENT: CONTRIBUTIONS OF DIRECT RELEASE AND RIVER DISCHARGE

Daisuke Tsumune^{a,*}, Takaki Tsubono^b, Kazuhiro Misumi^b, Kazuyuki Sakuma^c, Munehiro Asao^a, Yuko Hatano^a, Yuichi Onda^a

^a*University of Tsukuba*

^b*Central Research Institute of Electric Power Industry.*

^c*Japan Atomic Energy Agency*

**Corresponding author: tsumune.daisuke.gw@u.tsukuba.ac.jp*

Abstract

After the Fukushima Daiichi Nuclear Power Plant (F1NPS) accident, the oceanic ^{137}Cs activity concentration has not returned to the level before the accident. This is due to the continuous direct release from the F1NPS site and the river discharge of ^{137}Cs that has deposited on land. Understanding the dispersion process of ^{137}Cs in coastal areas is important for assessing the impact of these multiple sources. In this study, we estimated the contribution rates of direct release and river discharge by combining ocean dispersion simulations and analysis of observation data.

We conducted numerical simulations that considered direct release and river discharge and compared them with annual averaged observation data from 2013 to 2016[1]. The complex chemical behaviour of ^{137}Cs supplied from rivers to the ocean, such as aggregation, precipitation, dissolution, and resuspension, during the transition from freshwater to seawater, has not yet been clarified. In the simulation, it was assumed that the particulate ^{137}Cs discharged from the river would be resuspended and resolved within one year. By taking into account the river discharge[2], the reproducibility of the simulation was improved. Furthermore, the contribution ratios of direct release and river discharge were estimated. To verify the results of the contribution ratio estimation, the contribution ratios of ^{137}Cs at the observation point were estimated using the differences in the time series changes in the ^{137}Cs flux of direct release and river discharge. The time series analysis of the observation results showed a high correlation between the results of the contribution rate estimation for direct release and river discharge and the results of the simulation, confirming the validity of both methods. These results show that it is necessary to comprehensively analyse both direct release and river discharge in order to understand the diffusion of ^{137}Cs in coastal areas.

Keywords: ^{137}Cs , Fukushima Daiichi Nuclear Power Plant accident, Direct release, River discharge, Regional Ocean Model

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PLASTICS AND MICROPLASTICS IN THE MARINE ENVIRONMENT

Sakellariadou F

Dept of Maritime Studies, University of Piraeus, Piraeus, Greece.

**Corresponding author: fsakelar@unipi.gr*

Abstract

Plastics are synthetic or semi-synthetic organic polymers. Since the beginning of mass production of plastic products in the 1950s, plastic waste has accumulated in the terrestrial and marine environment endangering ecosystems and causing socio-economic impacts. Plastic pollution threatens human health through the presence of plastics found in, for example, blood, the brain and breastmilk¹.

In the sea, plastic pollution is present on the surface, throughout the water column and on the seabed. It is found in every marine region, from shallow coastal areas to the deepest regions as well as the most remote and fragile areas of the planet². By 2025, the amount of plastic in the seas is expected to total 150 million tonnes³. Biological effects include the injury and death. Common impacts are the ingestion, suffocation and entanglement of marine species. Plastics introduce a chemical risk through the leaching of a wide range of chemicals they contain and a variety of absorbed organic pollutants. They serve for the transportation and invasion of alien species. Plastic pollution causes a decrease of the ecosystem services.

Microplastics (<5mm) and nanoplastics (<1000nm) are created by the degradation of larger plastic products but are also produced in this size. Microplastic particles present in personal care and cosmetic products and microplastic fibers present in domestic sewage are not retained during sewage treatment and thus can enter the marine environment. Plastic degradation takes place via photo-oxidation and thermal reactions. At the deep seafloor, the degradation rate is quite low. Mainly land-based sources but also maritime activities, including ghost fishing gear, contribute to plastic pollution in the sea.

Transitioning to a safe, toxic-free circular plastics economy, adopting alternatives including biodegradable and compostable plastics, and implementing ensuring environmentally sound waste management practices are important tools to address the threat of plastic pollution.

Keywords: marine environment, plastic pollution

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MICRO- AND NANOPLASTICS IN ENVIRONMENTAL SAMPLES – REQUIREMENTS FOR RELIABLE QUANTIFICATION

Roland Kallenborn^{a,*}, Katrin Vorkamp^b

^a*Faculty of Chemistry, Biotechnology and Food Sciences (KBM); Norwegian University of Life Sciences (NMBU), Ås, Norway.*

^b*Department of Environmental Science, Aarhus University, Roskilde, Denmark*

**Corresponding author: Roland.kallenborn@nmbu.no*

Abstract

In recent years, the fate and distribution profiles of micro- and nanometer-sized organic polymeric materials (micro- and nanoplastics; MP/NP) have become a focus area in international environmental sciences. Quantification of MP is often based on spectroscopic methods, such as Fourier-Transform Infrared (FT-IR) and Raman spectroscopy. Restrictions in size resolution and contamination issues usually prevent the determination of particles smaller than 0.5 μm , thus excluding typical NP size fractions. An alternative quantification method is based on pyrolysis combined with gas chromatography/mass spectrometry (Pyr-GC/MS). Regardless of the analytical method, the quantitative polymer-specific analysis of MP/NP in the environment is crucial for understanding their sources, distribution and impacts on ecosystems and human health.

This presentation outlines the essential quality criteria for MP/NP analyses, emphasizing the need for harmonized methodologies and standardized quality assurance and control (QA/QC) measures to ensure accuracy and reproducibility. Key steps include sample collection and preparation, detection and identification, quality control (including representative blanks as well as positive controls/recovery), and standardized reporting for data interpretation. Several national and international monitoring programs have extended their efforts to include MP/NP. The Arctic Monitoring and Assessment Programme (AMAP) recently prepared a monitoring plan as well as monitoring guidelines, including QA/QC recommendations for coordinated and harmonized MP monitoring in the Arctic. The guidelines developed by AMAP will be discussed as a starting point for appropriate analytical strategies for MP/NP quantification. By adhering to appropriate quality control criteria, researchers and laboratories can improve the reliability of microplastic studies, contributing to more effective environmental management and mitigation strategies.

Keywords: Quantitative methods, Microplastic, environment, quality control



SOLID-STATE NMR SPECTROSCOPY HOW MISTRUST IN ITS RELIABILITY REVEALED NEW INSIGHTS IN SOIL BIOCHEMICAL PROCESSES

Heike Knicker^{a,*}

^a Group of Interactions between Soils, Plants and Microorganisms, Instituto de la Grasa (IG-CSIC), Sevilla, Spain

*Corresponding author: hekknicker@ig.csic.es

Abstract

With its introduction in the 1980's, solid-state NMR spectroscopy opened the door for a non-degradative analysis of soil organic matter (SOM). However, the obtained results were not always supporting well-accepted paradigms. Mistrust about its reliability survived up to our days, although already in its early days, fundamental studies could demonstrate that quantitative solid-state NMR data can be obtained if i) correct acquisition parameters are chosen, ii) the impact of paramagnetic compounds is reduced, and iii) the presence of soot in soils can be excluded. However, if in spite of following those prerequisites, NMR results are still in contrast with the expectations, it is most likely that the latter are wrong and a reassessment of even well-accepted views is required. As NMR spectroscopy has confronted me with this challenge more than once, I made it to the focus of my presentation, allowing me to share with the audience how this technique and its "misconduct" formed my understanding of function and nature of SOM. One example of such an event occurred during the investigation of the negative impact of paramagnetics on the quantification of NMR spectra. It turned out that carbohydrates are by far more important for organo-mineral interactions in soils than formerly thought. Another example derived from the intention to characterize charred residues by solid-state NMR spectroscopy. Formerly this was expected to be problematic due to the assumed graphenic nature of charcoal. However, the successful application of this approach to charcoals challenged this well-accepted view. More structural details about the molecular properties of pyrogenic organic matter were then deduced by two dimensional HETeronucleus CORelation ¹³C (HETCOR). Combined with relaxation time measurements, further information about H-C distances or molecular mobility can be achieved. Thus, applied in soil sciences, this approach offers a powerful tool to relate spatial molecular properties to soil biochemical processes.

In addition to the mentioned success story, the presentation will give me the opportunity to discuss pros and contras of solid-state NMR spectroscopy for SOM characterization hoping to demonstrate its value not only in soil sciences but also for studying processes in related research fields.

Keywords: Soil organic matter, 1D solid-state NMR, HETCOR, Cross polarization, Soil Biochemistry

NMR WITHOUT FOURIER TRANSFORM: A NEW ERA FOR ENVIRONMENTAL ANALYSIS BY NMR

Jeremy R. Gauthier^{a,*}, Andre J. Simpson^{a,b}, Scott A. Mabury^a

^aDepartment of Chemistry, University of Toronto, Toronto ON, Canada.

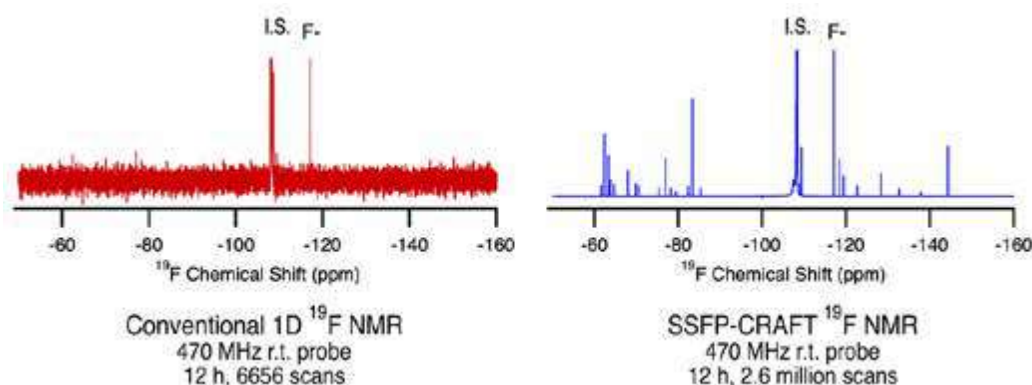
^bPhysical and Environmental Sciences, University of Toronto at Scarborough, Toronto ON, Canada

*Corresponding author: jeremy.gauthier@utoronto.ca

Abstract

A growing mass balance of unknown fluorine in environmental and biological samples is driving an urgent need for analytical techniques which can perform direct measurement and help identify unknown fluorinated compounds. ¹⁹F NMR demonstrates tremendous potential as it can solve structures without the use of libraries, leading to identification of new transformation products or classes of pollutants. However, NMR has traditionally been limited by relatively lower sensitivity in comparison with other analytical techniques. To address this sensitivity limitation, we employ steady-state free precession (SSFP) NMR alongside non-Fourier transform data analysis (CRAFT) to increase sensitivity of NMR as much as 20x that of a conventional 1D experiment.¹ SSFP can acquire hundreds to thousands of scans in very short experiment times, while CRAFT analysis overcomes limitations when working with severely truncated FIDs. The combined SSFP-CRAFT approach, applicable to almost any spectrometer or nuclei, reveals more fluorinated compounds than previously possible, often allowing for direct analysis in complex samples of trace concentration per- and polyfluorinated alkyl substances (PFAS). Across all samples including drinking water, human serum, agricultural biosolids, and polar bear liver, more fluorine resonances are detected, helping fill-in the unknown fluorine mass balance. Detection limits of NMR are lowered as much as 50x for the measurement of PFAS in human whole blood. The combined approach redefines the capability of ¹⁹F NMR as a screening tool for fluorinated compounds.

Keywords: NMR, environmental, analytical, PFAS, fluorine



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A TRANSPORTABLE MRI SENSOR TO MONITOR THE WATER STATUS OF PLANTS *IN SITU*

Guilhem Pagés^{a,b,*}

^aUniversité Clermont Auvergne, INRAE, UR QuaPA, 63122 Saint-Genès-Champanelle, France.

^bINRAE, PROBE Research Infrastructure, AgroResonance Facility, 63122 Saint-Genès-Champanelle, France.

*Corresponding author: guilhem.pages@inrae.fr

Abstract

Grasslands and forests play a crucial role in mitigating global warming due to their significant capacity to store carbon. Water is essential in this process, as it acts as a reactant in converting carbon dioxide into sugars during photosynthesis. In the context of global warming and climate change, understanding how plants manage water is critical. However, there is currently no sensor capable of locally probing water content and its movement directly in plants within their natural environment—i.e., *in situ*.

Magnetic resonance imaging (MRI) is the preferred analytical tool for non-invasive, localized measurement of water properties. To make these instruments transportable, low-magnetic-field devices have been developed,¹ including unilateral magnets.² With such unilateral instruments, the sample is placed at the magnet's surface, and the signal is recorded in a thin slice at a known distance from the surface. By precisely adjusting the magnet's position using a high-precision lift, a 1D image or profile can be obtained. This is the principle behind the NMR-MOUSE.³

Few portable devices have been used to study plant evolution *in situ*.⁴ In this work, we evaluated the potential of a unilateral MRI sensor to characterize the plant's water status directly *in situ*, both in the roots (underground) and branches (aboveground). Our results demonstrate that the measurements are quantitative and consistent across different plant species.⁵ Furthermore, through these non-invasive measurements, we were able to extract key indicators of the plant's water status.

Keywords: hydric stress, quantitative, rhizotron, tree, water

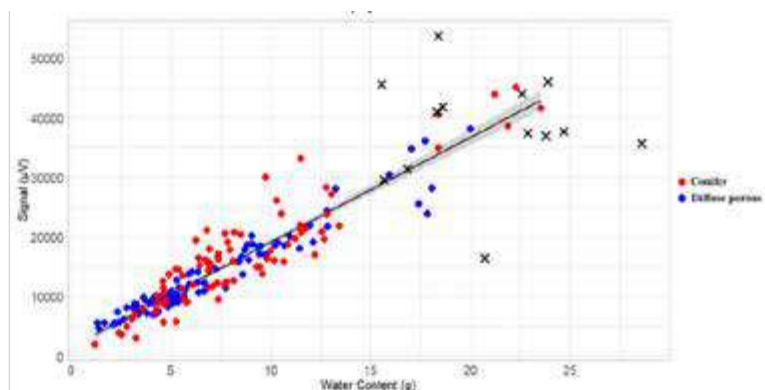


Figure: (Left) Example of an *in situ* measurement. The system is fixed on a vector to position the sensor against the tree. (Right) Relationship between MRI signal and the water quantity on *ex situ* branches (circles). A linear relationship was found. *In situ* tree measurements were performed (crosses).

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ILLITE MINERAL PHYSICOCHEMICAL TRANSFORMATION UPON NH₃ GAS TREATMENT

Di Pietro, S. A.^{a,*}, Mason, H. E.^b, Marple, M. A.^a, Sawvel, A. M.^a

^aLawrence Livermore National Laboratory, Livermore, California 94550, USA

^bLos Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

*Corresponding author: dipietro3@llnl.gov

Abstract

Application of reactive gases including ammonia (NH₃) is being considered for remediation of radionuclides by pH manipulation in unsaturated zones, such as those at the Department of Energy's (DOE) Hanford Site in Washington State. Ammonia gas injections may decrease radionuclide mobility without addition of liquid amendments into the vadose zone and quickly elevate the pH inducing soil mineral dissolution.¹ As NH₃ dissipates and the pH returns to neutral, co-precipitation processes are expected to occur between radionuclides and dissolved cations. However, the mineral dissolution and secondary precipitate formation processes are not well understood in these conditions.

The objective of this study was to investigate solid phase transformations due to the dissolution and precipitation of secondary minerals following treatment of pure mineral illite with NH₃ gas. Experiments were conducted using NH₄OH solutions as well as NaOH as comparable alkaline treatments while measuring pH and oxidation reduction potential (ORP) changes. Major cations (Si⁴⁺, Al³⁺, Ca²⁺, etc.) in the aqueous phase were monitored for over 60 days to determine the dissolved concentration from the solid phase with inductively coupled plasma mass spectroscopy (ICP-MS). In addition, solid samples were characterized using a variety of techniques, including solid state ²⁷Al and ²⁹Si nuclear magnetic resonance analysis, X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, and microscopy methods to investigate physicochemical transformations.

Results suggest major physicochemical changes of the phyllosilicate mineral (i.e., illite), particularly in the octahedral layers of the mineral. Structural changes in silicate ([SiO₄]ⁿ⁻) and aluminol (Al-OH) groups were identified by NMR and FTIR.² This research showed that mineral alteration processes occur during and after NH₃ gas treatment which may be used to remove radionuclides from the aqueous phase through sorption, co-precipitation, and coating with secondary phyllosilicate alteration products.

Keywords: environmental remediation, solid state nuclear magnetic resonance analysis, illite mineral, physicochemical transformation, phase characterization

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UNVEILING BIOCHAR-UREA INTERACTIONS IN SLOW-RELEASE NITROGEN FERTILIZERS: A MULTINUCLEAR SOLID STATE NMR STUDY

Silvia Pizzanelli^{a,*}, Elisa Carignani^a, Lucia Calucci^a, Claudia Forte^a, Daniel P. Rasse^b, Silvia Borsacchi^a

^a *Consiglio Nazionale delle Ricerche (CNR), Istituto di Chimica dei Composti OrganoMetallici (ICCOM)*

^b *Norwegian Institute of Bioeconomy Research (NIBIO), Department of Biogeochemistry and Soil Quality*

*Corresponding author: silvia.pizzanelli@cnr.it

Abstract

Composites constituted by urea and biochar are slow-release fertilizers expected to be particularly beneficial for the soil. The interaction between urea and biochar is a key aspect for the successful use of these composites, as it affects urea retention and subsequent release, and its understanding at a molecular level is a challenging task. In this work, multinuclear Solid State NMR (SSNMR) spectroscopy, also combined with the use of ^{13}C and ^{15}N isotopically enriched urea, was employed to get insight into urea-biochar interactions.¹ Composites were prepared according to two different impregnation methods, one based on saturated aqueous urea solution and the other on molten urea, resulting in the BUs and BUm composites, respectively. ^{13}C and ^{15}N SSNMR experiments carried out on the composites before and after release in water at different times revealed that urea predominantly exists in the composites in the paracrystalline form on the surface of biochar or physically entrapped within biochar pores. In BUm, products of thermal degradation of urea were also detected, mainly in the form of biuret. Release experiments showed 78% and 64% loss of urea, for BUs and BUm, respectively, after 24 hours of immersion in water. Notably, residual urea is mainly physically confined in the biochar pores. In the case of BUm, species arising from the thermal degradation of urea are also partially retained. The adopted comprehensive characterization methodology elucidated the impact of the preparation method on the composition and the release behavior of the composites and offered an unprecedented view of the interactions between urea and biochar at the molecular level.

Keywords: biochar-based fertilizers, sustainable agriculture, ^{13}C and ^{15}N MAS NMR, urea thermal degradation, entrapped urea.

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NEXT-GENERATION MATERIALS FOR GAS SEPARATION AND CARBON CAPTURE: INSIGHTS FROM SOLID STATE NMR SPECTROSCOPY

Francesca Martini^{a,*}, Elisa Della Latta^a, Francesca Nardelli^a, Marco Geppi^a, Lucia Calucci^b

^a*Dipartimento di Chimica e Chimica Industriale, Università di Pisa (Italia)*

^b*Istituto di Chimica dei Composti Organometallici, Consiglio Nazionale delle Ricerche, Pisa (Italia)*

*Corresponding author: francesca.martini@unipi.it

Abstract

The development of next-generation materials for gas separation is crucial for enhancing energy efficiency and reducing the environmental impact of industrial processes. Traditional gas separation methods, such as cryogenic distillation and adsorption-based techniques, often require high energy consumption and complex operational setups. In contrast, membrane-based technologies offer a more sustainable and cost-effective alternative, enabling continuous, scalable, and energy-efficient gas separation. Advanced membrane materials, such as Metal-Organic Frameworks (MOFs)^{1,2} and Covalent Organic Frameworks (COFs),³ offer superior selectivity and permeability due to their tunable porosity and chemical functionality, yielding excellent results in selective CO₂ separation, capture, and hydrogen purification. Additionally, Polymers of Intrinsic Microporosity (PIMs),^{4,5} with their rigid and highly porous structures, exhibit remarkable gas transport properties, while Mixed-Matrix Membranes (MMMs)⁶ integrating MOFs or graphene-based fillers further enhance separation performance. Solid-state NMR spectroscopy plays a key role in characterizing these materials at the atomic level,^{7,8,9} offering insights into their molecular interactions, structural stability, as well as their adsorption and transport mechanisms. In this contribution, I will present some recent applications of solid-state NMR spectroscopy for studying gas separation materials, with examples drawn from studies conducted in my research group in Pisa.

PRIN PNRR 2022 “In MoTion-Influence of dynaMics on the adsorption and Transport properties in polymeric materials for membrane technologies” funded by the European Union - Next Generation EU is acknowledged for financial support.

Keywords: gas separation, carbon dioxide, membranes, MOFs, solid state NMR, structure and dynamic characterization

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CATCHING POLLUTANTS WITH SELENADIAZOLE FUNCTIONALISED PORPHYRIN NANOTUBES

Catriona Thomson¹, Marc-Antoine Sani² and Jonathan White^{1,*}

¹ School of Chemistry, University of Melbourne, Melbourne, VIC 3010, Australia

² Bio21 Institute, University of Melbourne, Melbourne, VIC 3010, Australia

*Corresponding author: whitejm@unimelb.edu.au

Abstract

Chalcogen bonding is an attractive non-covalent interaction which remains relatively under-explored in terms of its applications in supramolecular chemistry. This work presents a material with chalcogen bond donor units capable of engaging in host-guest interactions with Lewis Basic guests. These materials have high potential in developing capture systems for pollutants found in wastewater and chemical management. Utilising the structural rigidity of the tetrakis(4-pyridyl)porphyrin molecule, we recently reported a novel porous crystalline porphyrin nanotube (PNT) which self-assembles as discrete, hexagonal one-dimensional porous coordination polymers (PCPs) (Figure 1).¹ Revealed by Single Crystal X-ray Diffraction (SCXRD) data, each nanotube encloses a large one-dimensional channel running through the crystallographic *c*-axis, with a pore diameter greater than 10 Å, a void volume comprising 35 % of the unit cell and key chalcogen bonding functionality lining the voids. To investigate the capacity of PNT to participate in chalcogen bonding with guest molecules, crystals of desolvated PNT were immersed in d₆-DMSO. Solid-state ⁷⁷Se, ¹³C, ¹¹³Cd, and ²H NMR, in conjunction with gas sorbance experiments, identified the molecular affinity of PNT for d₆-DMSO, the mode of motions within the PNT scaffold and the behavior of the host-guest interaction across a wide range of temperature. Deuterium line shape simulations deduce 3 primary motions of d₆-DMSO guest molecules. There are two intramolecular rotations (namely the C3 rotation of methyl groups and C2 rotation about the mirror plane of the molecule) and one intermolecular C6 hopping motion about the selenadiazole sites lining the pores of PNT. The variation in temperature induced a slight alteration of the space hosting the DMSO and hence the guest molecules' motions within the nanotube. Broadening the type of guests that may be taken up by the PNT is another area offering exciting opportunities for further investigation.

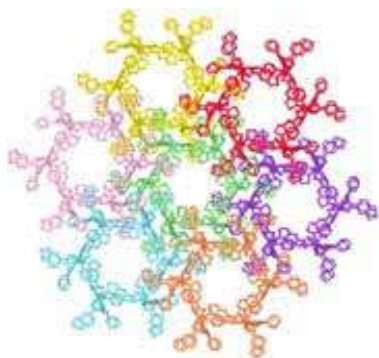


Figure 1. Hexagonal packing of PNT

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VARIATIONS IN SOIL ORGANIC MATTER COMPOSITION OF TROPICAL PEATLAND IN SARAWAK, MALAYSIA USING ^{13}C NMR SPECTROSCOPY

Nur Azima Busman^{a*}, Lulie Melling^a, Faustina E. Sangok^a and Akira Watanabe^b

^a*Sarawak Tropical Peat Research Institute, Kota Samarahan, Sarawak, Malaysia*

^b*Graduate School of Bioagricultural Sciences, Nagoya University, Nagoya, Japan*

*Corresponding author: nurazima.b@sarawak.gov.my

Abstract

Tropical peat swamp forests in Sarawak are characterized by different forest types that vary in their vegetation, topography, and hydrology, which influence the formation and composition of soil organic matter (SOM). In this study, the chemical structure of SOM in three distinct forest types; Mixed Peat Swamp (MPS), Alan Batu (ABt), and Alan Bunga (ABg), was analyzed using solid-state ^{13}C nuclear magnetic resonance (NMR) spectroscopy. The main objective was to assess the stability of SOM and its susceptibility to land use change. Soil samples were collected from depth gradients in each forest type and analyzed to determine the distribution of carbon functional groups. The MPS soils showed a decrease in alkyl C and an increase in *O*-alkyl C with increasing soil depth, indicating progressive decomposition. In contrast, SOM composition in ABt and ABg soils remained relatively stable across depths, with higher aromatic C content, indicating a slower rate of decomposition. To simulate the effects of land use change, a five-year incubation was carried out under drained conditions. The ^{13}C NMR analysis revealed that carbon loss was significantly influenced by the initial SOM composition, i.e. soils with a higher *O*-alkyl C content had a greater C loss. The changes in SOM composition after incubation were small, but the results suggest that stable components such as alkyl C and aromatic C may also decrease alongside labile carbon such as *O*-alkyl C with prolonged drainage. Overall, this study highlighted the variability of SOM composition across different forest types and their sensitivity to drainage and land use change. Solid-state ^{13}C NMR spectroscopy proves to be an effective tool for characterizing SOM in tropical peatlands. These findings are crucial for the sustainable management of peatlands and for conservation strategies aimed at minimizing carbon loss and supporting environmental sustainability.

Keywords: ^{13}C NMR spectroscopy, carbon loss, land use change, soil organic matter, tropical peatland

BRIDGING THE GAP BETWEEN THE ENVIRONMENTAL IMPACTS OF TYRE PARTICLES, TYRE RECOVERY AND END-OF-LIFE SOLUTIONS

Dr Linda Mitchell^{a,*}, Lina Goodman^a

^a Tyre Stewardship Australia.

*Corresponding author: linda.mitchell@tyrestewardship.org.au

Abstract

Tyres are a crucial product in modern society, essential for global mobility, mineral extraction, and resource production. Given the sheer volume of tyres, it is important to understand the varying environmental impacts during their use, recovery, and reuse in new products. This discussion will explore key challenges across the tyre value chain which require further understanding, to drive sustainable solutions whilst minimising environmental harm.^{1,2}

A major challenge for tyres is the production of tyre and road wear particles, which can release chemicals of concern, as well as impact the surrounding environment. Considerable research efforts are underway to limit tyre abrasion, find safer chemical alternatives, and develop mitigation strategies to reduce pollution. These activities often face competing priorities within the tyre industry, such as the shift towards more sustainable materials and the development of fuel-efficient tyres.

Tyres reaching their end-of-life also face many challenges, and poor management can lead to considerable dumping and stockpiling, a dramatic loss of valuable resources. Mismanaged tyres can provide breeding habitats for mosquitoes, vermin, and can cause major fires, which have devastating impacts on the environment.

Globally, tyre management approaches aim to improve the recovery rates of used tyres whilst reducing environmental harm. In Australia, there is considerable focus on driving circular economy outcomes for tyres, particularly via research into valuable market products. The development of tyre-derived products also requires a consideration for potential downstream environmental impacts. Given these products are distinct from their first life counterparts, they require unique approaches to understand and manage these impacts.

Environmental challenges are different between each stage of a tyre lifecycle, yet there is an opportunity to work collaboratively and find multifaceted solutions. A circular economy for tyres will include solutions which minimise waste and pollution across the value chain, while also recirculating materials at their highest value.

Keywords: tyre particles, end-of-life tyres, circular economy, environmental impact, resource recovery

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ENVIRONMENTAL DEGRADATION AND IMPACT ASSESSMENT OF TIRE-DERIVED MICROPLASTICS: A COMPARATIVE STUDY OF UNUSED TIRES, RECYCLED RUBBER CHIPS, AND TIRE AND ROAD WEAR PARTICLES

Daryll Anne Dimapilis^a, Hiroshi Sakai^a, Dilraj Surendran^a, Shogo Takagi^a

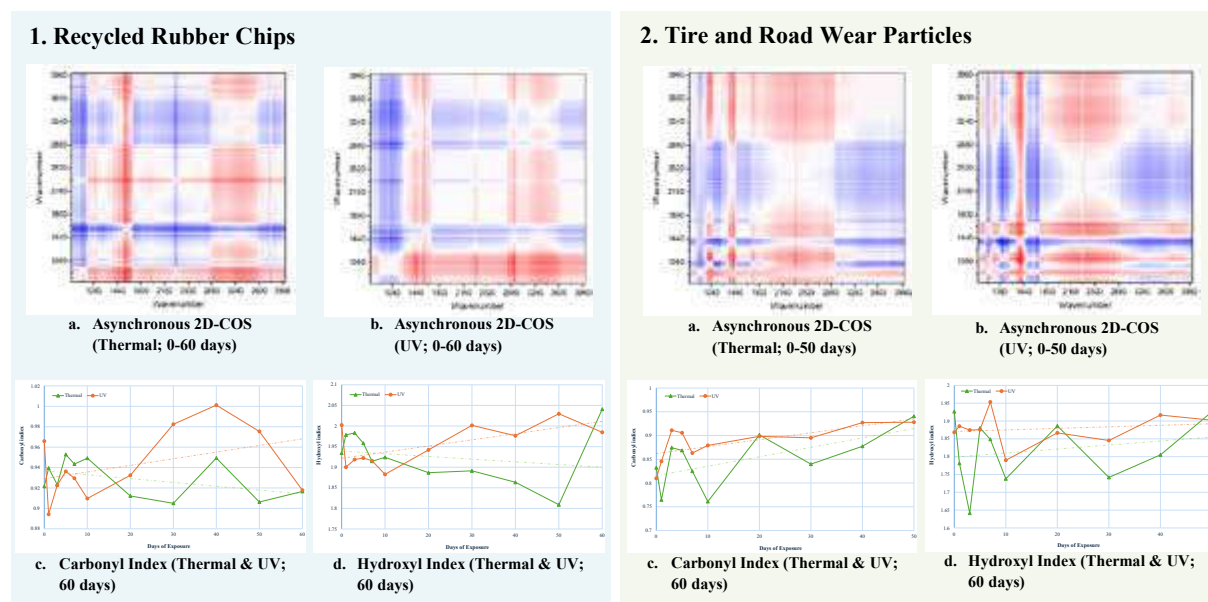
^aDepartment of Civil and Environmental Engineering, Tokyo Metropolitan University, Japan

*Corresponding author: dimapilis-anne@ed.tmu.ac.jp

Abstract

Tire-derived microplastics, including Recycled Rubber Chips (RRC) and Tire and Road Wear Particles (TRWP), are emerging as significant environmental pollutants. This study investigates the degradation of RRC and TRWP under thermal and UV exposure over 60 days. FTIR spectra were collected to analyze changes in functional groups, and 2D-COS analysis was performed to track the degradation patterns. Mass loss was also monitored as an indicator of degradation. During thermal degradation, both materials showed the formation of vinyl groups and unsaturated bonds due to scission in the rubber backbone, with plasticizers depleting and C-O bonds hydrolyzing or volatilizing in the early stages (0–5 days). By day 5, oxidation of the sulfur network led to the formation of sulfoxides and the breakdown of nitrile-based antioxidants. Thermal degradation resulted in a steady breakdown of the polymer network, with complete degradation of C-S bonds by day 60, particularly for TRWP. UV exposure caused radical formation at weak C-H bonds, leading to aliphatic chain scission and volatile compound release. By days 5–20, hydroxyl groups and unsaturated C=C structures formed, with significant additive leaching, especially in RRC. UV degradation progressed more rapidly than thermal degradation, with RRC exhibiting faster breakdown and higher microplastic release compared to TRWP. Both materials showed an increase in carbonyl and hydroxyl indices, indicating accelerated oxidation, with the effect more pronounced in RRC than in TRWP. The mass loss patterns also differed, with UV-exposed samples degrading quickly at first, followed by stabilization, while thermal degradation resulted in slower, continuous breakdown. These findings suggest that TRWP, which has already been exposed to environmental aging, may persist longer in the environment, while RRC degrades faster, releasing by-products more quickly. Understanding these degradation mechanisms helps assess the long-term environmental risks of tire-derived microplastics and guide pollution control and sustainable tire production strategies.

Keywords: tire-derived microplastics, tire and road wear particles, rubber, FTIR, 2D-COS



FATE AND TRANSPORT OF TOXIC CHEMICALS LEACHING FROM TYRE WEAR PARTICLES

Rai Kookana and Divina Navarro

The University of Adelaide/ CSIRO Environment, Waite Campus, Urrbrae, Australia 5064

**Corresponding author: Kookana@gmail.com*

Abstract

Millions of tonnes of tyre wear particles (TWPs), containing a complex mix of organic and inorganic chemicals, are released into the environment each year. Among these, the tyre additive 6PPD (N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine) and its oxidation product 6PPD-quinone (6PPD-q) are of particular concern due to their high toxicity to a wide range of aquatic organisms, especially fish. Effective mitigation measures depend on understanding the environmental fate and transport of TWPs and the associated chemicals. Surface runoff and stormwater are the primary pathways through which TWPs and their leached chemicals enter natural water bodies and treatment systems. Both 6PPD and 6PPD-q are sufficiently soluble to travel in dissolved form and hydrophobic enough to adhere to suspended particles, allowing for transport via water and solids both. A clearer understanding of the partitioning between dissolved and particulate fractions of 6PPD and 6PPD-q is critical for assessing environmental exposure. Both compounds have been detected in drinking water sourced from surface waters; one study found 6PPD-q in 100% of filtered river water samples at low (ng/L) concentrations. Bioretention systems have shown potential in reducing the mass loading of these contaminants to receiving waters. While conventional wastewater treatment significantly reduces their concentrations, their strong affinity for organic matter results in their accumulation in biosolids. The application of biosolids to agricultural land may thus pose a risk to soil organisms. Major knowledge gaps remain in our understanding of the fate, transport, and long-term impacts of TWPs and their associated chemicals.

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CHEMINFORMATICS DRIVING SUSTAINABLE SOLUTIONS: INTEGRATING MOLECULAR MODELING AND SIMULATIONS, AI, AND QUANTUM COMPUTING IN HEALTHCARE, ENERGY, AND ENVIRONMENTAL SCIENCES

Vannajan Sanghiran Lee

Department of Chemistry, Center of Excellence for Quantum Information Science and Technology (QIST), Faculty of Science, University Malaya, Kuala Lumpur 50603, Malaysia and

Center of Excellence in Structural and Computational Biology, Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

Corresponding author: vannajan@um.edu.my, vannajan@gmail.com

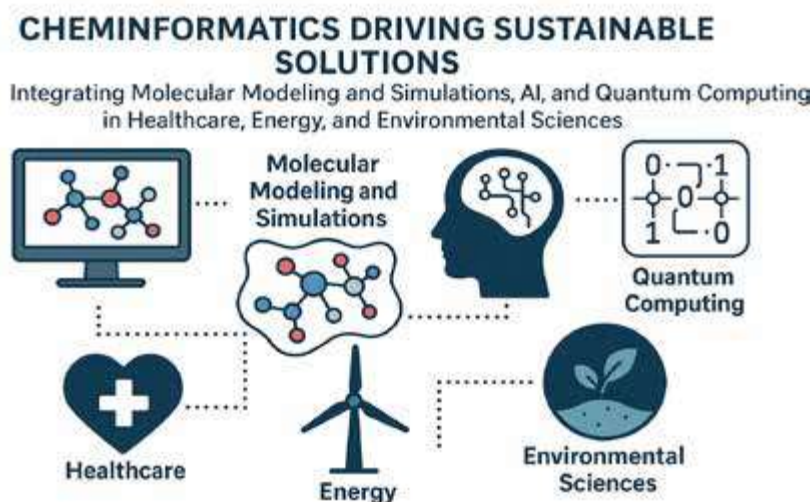
Abstract

Cheminformatics, the integration of computational techniques to address chemical challenges, is rapidly evolving through its fusion with artificial intelligence (AI), machine learning (ML), and quantum computing. This interdisciplinary convergence is accelerating breakthroughs across healthcare, energy, and environmental sectors, where complex molecular systems demand advanced modeling and simulation.

In healthcare, AI-driven cheminformatics enables high-throughput virtual screening, QSAR modelling, and predictive analytics for drug discovery. Molecular dynamics (MD) simulations provide detailed insights into biomolecular interactions and thermodynamic stability, while quantum computing simulates molecular structures and reaction pathways with high accuracy, advancing drug design and precision medicine. In the energy sector, these technologies streamline the design of advanced materials for batteries, fuel cells, and catalysts. AI and cheminformatics optimize compound identification, while MD simulations reveal ion diffusion and transport mechanisms, with quantum simulations deepening our understanding of electron transfer and energy conversion processes. In environmental science, AI and cheminformatics facilitate modelling of pollutants and risk assessment, while MD simulations model molecular transport, and quantum chemistry aids in predicting degradation pathways, supporting the design of effective remediation strategies.

This keynote will explore how the synergy of cheminformatics, molecular modelling and simulations, AI, and quantum computing is advancing scientific discovery, aligning with global sustainability goals, and offering transformative solutions for healthcare, energy, and environmental challenges.

Keywords: Cheminformatics, Molecular modelling and simulations, Artificial intelligence (AI), Quantum technology, Sustainable innovation



NEXT-GEN FLUID MODELING: PREDICTING CRITICAL PROPERTIES, ACENTRIC FACTORS, AND BOILING POINTS OF PURE FLUIDS WITH ENSEMBLE LEARNING

Roda Bounaceur^a, Romain Privat^a, Francisco Paes^a, Jean-Noël Jaubert^{a,*}

^aUniversité de Lorraine, CNRS, LRGP, F-54000 Nancy, France

*Corresponding author: jean-noel.jaubert@univ-lorraine.fr

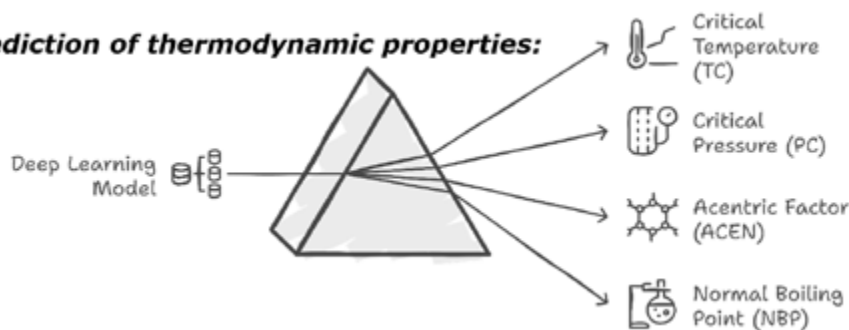
Abstract

For a pure fluid, an equation of state (EoS) is a mathematical expression that relates pressure, temperature and molar volume. It provides a means to perform fluid phase equilibrium calculations, thereby enabling the estimation of vapor pressures, boiling points and property changes during vaporization. When coupled with a mathematical expression for the ideal gas heat capacity, an EoS can also estimate changes in enthalpy, entropy and exergy. EoS are thus a key component of any industrial process simulator. Among the numerous EoS available in the open literature, cubic EoS play a pivotal role because they can be straightforwardly parameterized and are very accurate when applied to non-associating fluids¹. For example, the most well-known cubic EoSs are those of Peng-Robinson and Redlich-Kwong-Soave. The input parameters for these EoSs are the critical temperature (T_c), the critical pressure (P_c) and the acentric factor (ω). When these properties are not available experimentally, they must be estimated with a high degree of accuracy.

For this reason, an ensemble learning technique that combines several machine learning algorithms has been developed to estimate T_c , P_c and ω for any compound comprising C, H, O, N, S, P, F, Cl, Br and I atoms. The open-source library MORDRED, developed in Python, was used to generate over 1,800 molecular descriptors to characterize the compounds studied. The learning database consists of experimental values for more than 1,700 molecules belonging to numerous chemical families. The accuracy of the proposed model has been tested on a wide range of experimental data and compared with that of various learning models recently reported in the literature. Such a comparison demonstrates the improved accuracy achieved by using the proposed model, which is why a tool was developed and distributed for estimating T_c , P_c and ω from the SMILES (Simplified Molecular Input Line Entry System) notation of a molecule. It is available free of charge at: <https://bioscope.streamlit.app/>

Keywords: critical properties, ensemble learning, artificial neural network, QSPR, molecular descriptors

AI prediction of thermodynamic properties:



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ALZYFINDER: A MACHINE-LEARNING-DRIVEN PLATFORM FOR LIGAND-BASED VIRTUAL SCREENING AND NETWORK PHARMACOLOGY

Jessica Valero-Rojas^{a,b}, Camilo Ramírez^c, Laura Pacheco-Paternina^a, Paulina Valenzuela-Hormazabal^a, Paula Santana^d, Janneth González^e, Tatiana Gutiérrez-Bunster^f, Alejandro Valdés-Jiménez^f, David Ramírez^{a,*}

^a Departamento de Farmacología, Facultad de Ciencias Biológicas, Universidad de Concepción, Concepción, Chile

^b Facultad de Ciencias Químicas, Universidad de Concepción, Concepción, Chile.

^c Facultad de Ingeniería, Diseño e Innovación, Institución Universitaria Politécnico Gran Colombiano, Bogotá, Colombia.

^d Facultad de Ingeniería, Instituto de Ciencias Aplicadas, Universidad Autónoma de Chile, Santiago Chile

^e Departamento de Nutrición y Bioquímica, Facultad de Ciencias, Pontificia Universidad Javeriana, Bogotá, Colombia.

^f Departamento de Sistemas de Información, Universidad del Bío-Bío, Concepción, Chile

*Corresponding author: dramriezs@udec.cl

Abstract

Alzheimer's disease (AD), a prevalent neurodegenerative disorder, presents significant challenges in drug development due to its multifactorial nature and complex pathophysiology ¹ISSN: "19994923", "abstract": "Neurodegenerative diseases (NDD. The AlzyFinder Platform ², addresses these challenges by providing a free web-based tool for parallel ligand-based virtual screening (LBVS) and network pharmacology, specifically targeting over 85 key proteins implicated in AD. This innovative approach is designed to enhance the identification and analysis of potential multitarget ligands. AlzyFinder incorporates machine learning models to facilitate the LBVS process. These models were meticulously trained and validated using robust methodologies to ensure high predictive accuracy. Validation included extensive testing with active, inactive, and decoy molecules, demonstrating the platform's efficacy in distinguishing active compounds. The models are evaluated based on balanced accuracy, precision, and F1 score metrics. A unique soft-voting ensemble approach is utilized to refine the classification process, integrating the strengths of individual models. This methodological framework enables a comprehensive analysis of interaction data, which is presented in multiple formats such as tables, heat maps, and interactive Ligand-Protein Interaction networks, thus enhancing the visualization and analysis of drug-protein interactions. AlzyFinder was applied to screen five molecules recently reported ³⁻⁷ (and not used to train or validate the ML models) as active compounds against five key AD targets. The platform demonstrated its efficacy by accurately predicting all five molecules as true positives with a probability greater than 0.70. This result underscores the platform's capability in identifying potential therapeutic compounds with high precision. In conclusion, AlzyFinder's innovative approach extends beyond traditional virtual screening by incorporating network pharmacology analysis, thus providing insights into the systemic actions of drug candidates. This feature allows for the exploration of ligand-protein and protein-protein interactions and their extensions, offering a comprehensive view of potential therapeutic impacts. AlzyFinder is available at <http://www.alzyfinder-platform.udec.cl> with supporting data and scripts accessible via GitHub <https://github.com/ramirezlab/AlzyFinder>.

Keywords: Ligand-Based Virtual Screening, Machine Learning, Alzheimer's disease, Network pharmacology, Cheminformatics.

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The diagram illustrates the Alzy Finder workflow for identifying Alzheimer's disease key targets, consisting of three main steps:

- Step 1: Input Data Collection**
 - Alzheimer's disease key targets:** A brain icon with a red box highlighting a specific region, leading to a detailed view of three protein targets: Ion channel, GPCR, and Kinase.
 - Ligands:** A collection of various chemical structures (red, blue, green, and purple) representing potential ligands.
- Step 2: Virtual Screening**
 - The workflow uses the **Alzy Finder** platform to perform virtual screening on the input data.
- Step 3: Output and Network Analysis**
 - Virtual screening heatmap:** A heatmap showing the results of the screening. The y-axis lists AD key targets (A, B, C, D) and the x-axis lists ligands (1, 2, 3, 4, 5, 6, 7). The color scale represents 'Active probability' from 0 (yellow) to 1 (dark red).
 - Ligand-Protein Interaction network:** A network diagram showing interactions between ligands (nodes) and proteins (edges). The nodes are color-coded by type: Ion channel (red), GPCR (blue), and Kinase (green). The edges are color-coded by type: Ion channel - GPCR (red), GPCR - Kinase (blue), and Ion channel - Kinase (green).

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TRANSLATING ORGANIC SPECTRA TO MOLECULAR STRUCTURES VIA CHEMIST-INSPIRED KNOWLEDGE INJECTION

Zhiyuan Yan^{a†}, Chengchun Liu^{b†}, Li Yuan^{a*}, Fanyang Mo^{b,c,d*}

^a School of Electronic and Computer Engineering, Peking University, No.2199 Lishui Road, Nanshan District, Shenzhen, 518055.

^b School of Materials Science and Engineering, Peking University, No.5 Yiheyuan Road, Haidian District, Beijing, 100871.

^c School of Advanced Materials, Peking University Shenzhen Graduate School, No.2199 Lishui Road, Nanshan District, Shenzhen, 518055.

^d Guangdong Provincial Key Laboratory of Nano-Micro Materials Research, Peking University Shenzhen Graduate School, No.2199 Lishui Road, Nanshan District, Shenzhen, 518055.

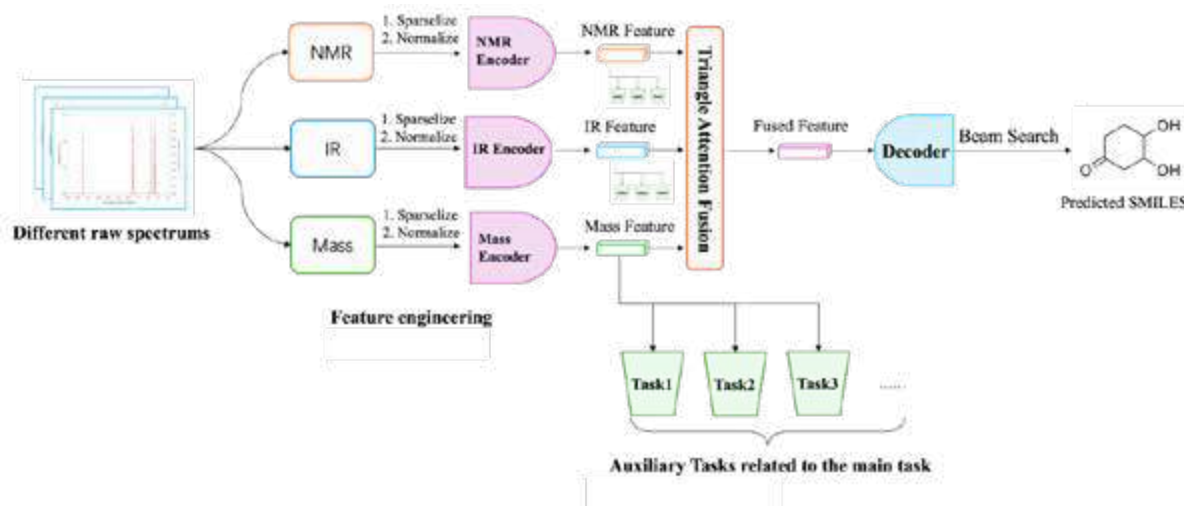
[†]These authors contributed equally to this work

*Corresponding author: yuanli-ece@pku.edu.cn; fmo@pku.edu.cn

Abstract

Elucidating the structure of a chemical compound is a fundamental task in chemistry, with applications in drug discovery, precision medicine, and biomarker discovery. Typically, chemists derive molecular structures by obtaining diverse organic spectra through experiments or computations and leveraging their domain knowledge. However, this process can be resource-intensive, slow, and highly dependent on the expertise of individual chemists. A promising approach to accelerate and simplify this task is through deep learning. However, two key challenges remain: First, there is a lack of a benchmarking dataset that includes diverse organic spectra for each molecule. Second, previous works mainly focus on single spectra, which provide limited information about the molecular structure and fail to capture the complex relationships between different spectra. To address these challenges, we propose a new benchmark using diverse spectra from the commonly used QM9 dataset, which includes infrared, mass, and NMR spectra for each molecule. Inspired by the way chemists' reason through spectra, we embed their domain knowledge into deep learning models by designing tailored feature engineering and introducing related auxiliary tasks. This enables the models to uncover and leverage the intricate clues hidden within each spectrum, just as a chemist would. Our results are striking: our approach achieves chemist-level accuracy on both academic and experimental datasets, paving the way for generalizing to novel and previously unseen molecules with unprecedented efficiency.

Keywords: infrared spectroscopy; knowledge embedding; interpretable machine learning



METHODS AND APPLICATIONS OF CHEMOINFORMATICS IN PESTICIDE DESIGN

Wenli Xu, Shuyang Jiang, Guohua Liu, Caiyan Yue, Jia Li, Ping Xing, Biao Jiang*, Jianhua Yao*

State Key Laboratory of Fluorine and Nitrogen Chemistry and Advanced Materials, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai, 200032, China.

**Corresponding author: yaojh@sioc.ac.cn, jiangb@sioc.ac.cn*

Abstract

Cheminformatics (also termed as cheminformatics and chemical informatics) is an application of informatics methods to solve the chemical problems concerned with molecular design, synthesis design and structural identification [1]. It is an interdisciplinary [2] combining of Computer science, Mathematics and Chemistry. These *in silico* techniques are used in, for example, pharmaceutical companies in the process of drug discovery. These methods can also be used in chemical and allied industries in various other forms. In principle, three methods are included in Chemoinformatics: data-based, logic-based and principle-based. They are used at different stage and different levels in chemical study. In November 2010, by FAO and WHO, the term “Pesticide” was defined as: to embrace active ingredients in any form, irrespective of whether, or to what extent, they have been formulated for application. The term is usually associated with materials intended to kill or control pests (insecticides, fungicides, herbicides, etc.) but, for the present purposes, it also embraces certain materials to control the behavior or physiology of pests (e.g. insect repellents and insect growth regulators) or of crops during production or storage. [3]. Obviously, pesticide has close relationships with chemistry, environment, ecology, biology, food safety, public health, toxicology and etc.

In Chemistry, molecular design, synthesis design and structural identification are included in pesticide design. Herein, some strategies, methods and applications of Chemoinformatics used in pesticide design will be presented.

Keywords: Chemoinformatics, Data-based, Logic-based, Principle-based, Pesticide design

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MULTIMODAL AI-DRIVEN MOLECULAR DESIGN OF ORGANIC REDOX MATERIALS FOR AQUEOUS REDOX FLOW BATTERIES

Sohyeon Lee^a, Yoonseok Lee^a, Jaehyeok Yang^a, Changseop Kim^a, Gyungmin Hwang^b, Daewon Chung^{a*}, Joonhyeon Jeon^{a,b*}

^aDepartment of Advanced Battery Convergence Engineering, Dongguk University-Seoul, Korea.

^bDivision of Electronics & Electrical Engineering, Dongguk University-Seoul, Korea

*Corresponding author: jung1362@dongguk.edu, memory@dgu.edu

Abstract

Redox-active organic materials are gaining attention as a safe and sustainable energy solution, with aqueous organic redox flow batteries (AORFBs)¹. However, finding active compounds with high solubility requires tedious and time-consuming computational and experimental processes. Recently, deep learning-based generative models using computer-aided molecular design are suggested as an efficient solution². Nevertheless, existing models lack flexibility, making it difficult to simultaneously satisfy multiple properties, thereby reducing efficiency in targeted molecular generation. To address this issue, this paper proposes an effective conditional generative adversarial network (cGAN) capable of generating molecules with desired physicochemical properties. As a simulation result, the proposed model is shown to generate molecules satisfying seven target properties at the same time, including structural characteristics (e.g., presence of halogen groups, number of aromatic rings) and physicochemical properties (e.g., penalized log P). The model generated valid molecular structures based on PubChem integrated database with a 65.8% success rate. When the log P, one of the parameters determining the solubility of a substance, was specified, the model demonstrated excellent performance in screening redox-active materials. This approach provides a new insight in developing AORFB active materials with various molecular properties.

Acknowledgments This work was supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP), and the Ministry of Trade, Industry & Energy (MOTIE) of the Republic of Korea (No. 20224000000020). This work was also supported by the Ministry of Science and ICT (MSIT), Korea, under the ICT Challenge and Advanced Network of HRD (ICAN) support program (IITP-2024-RS-2024-00437186), supervised by the Institute for Information & Communications Technology Planning & Evaluation (IITP).

Keywords: AORFB, electrolyte, molecule generation, multimodal learning, chemical information

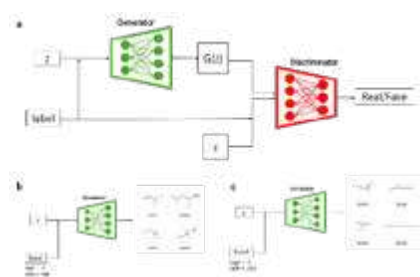


Fig.1. (a) is the proposed cGAN structure, and (b) and (c) are examples of molecule generation for different targets based on physicochemical properties.

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RATIONAL DESIGN OF MULTITARGET COMPOUNDS FOR ALZHEIMER DISEASE: A COMPUTATIONAL AND EXPERIMENTAL APPROACH

Jessica Valero-Rojas^{a,b}, Paulina Valenzuela-Hormazabal^a, Jhon J. López^b, David Ramírez^{a,*}

^a Pharmacology department, Faculty of Biological Sciences, University of Concepción, Concepción.

^b Organic Chemistry department, Faculty of Chemical Sciences, University of Concepción, Concepción.

*Corresponding author: dramirezs@udec.cl

Abstract

Alzheimer's disease (AD) is a common form of dementia characterized by the accumulation of β -amyloid ($A\beta$), resulting in the formation of plaques and neurofibrillary tangles (NFTs)¹, which lead to inflammation and disrupt neuronal function². Different hypothesis has been developed to explain this pathology, including: the amyloidogenic hypothesis, the NFTs, and the cholinergic hypothesis. Although the FDA has approved six drugs, donepezil, rivastigmine, galantamine, memantine, lecanemab, and aducanumab, for symptomatic treatment, an effective therapy for this multifactorial disease remains elusive³. Consequently, there is an urgent requirement to develop therapeutic strategies that simultaneously target the multiple pathological mechanisms underlying the disease.

This project explores the design of multitarget-directed ligands (MTDLs) for AD through an coupled computational and experimental pipeline. The main objective is to design and synthesize compounds capable of modulating multiple key targets in AD pathophysiology, including acetylcholinesterase (AChE), beta-secretase 1 (BACE-1), cannabinoid receptor type 2 (CB2), glycogen synthase kinase 3 beta (GSK-3 β), monoamine oxidase A (MAO-A), and nicotinic receptor alpha 7 (Rn- α 7)⁴.

First, we designed a $\sim 14 \times 10^6$ chemolibrary using commercial databases, followed by pharmacophore-based virtual screening and molecular docking to ultimately identifying 21 promising candidates for experimental validation. During the experimental phase, four compounds showed significant activity, with Z2119960793 (from Enamine Store) standing out as a particularly notable MTDLs against both AChE ($IC_{50} = 8.84 \pm 0.04 \mu M$) and GSK-3 β ($IC_{50} = 4.19 \pm 0.5 \mu M$) key AD targets.

Finally, the synthesis of compound Z2119960793 was carried out in our laboratory, achieving an 80% yield through the Steglich reaction. As part of future projections, 20 analogs of Z2119960793 are being designed, which will be experimentally evaluated against the enzymes AChE and GSK3B, as well as analyzed for their neuroprotective and neurotoxic potential.

Keywords: Alzheimer's disease; drug discovery; Multi-Target Directed Ligands; therapeutic targets; computational methods.

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APPLICATION OF A UNIVERSAL NEURAL NETWORK POTENTIAL FOR CO ADSORPTION ON SUPPORTED NANOPARTICLE CATALYSTS

Gerardo Valadez Huerta^{a,*}, Susan Meñez Aspera^a, Yusuke Nanba^a, Kaoru Hisama^a,
 Michihisa Koyama^a

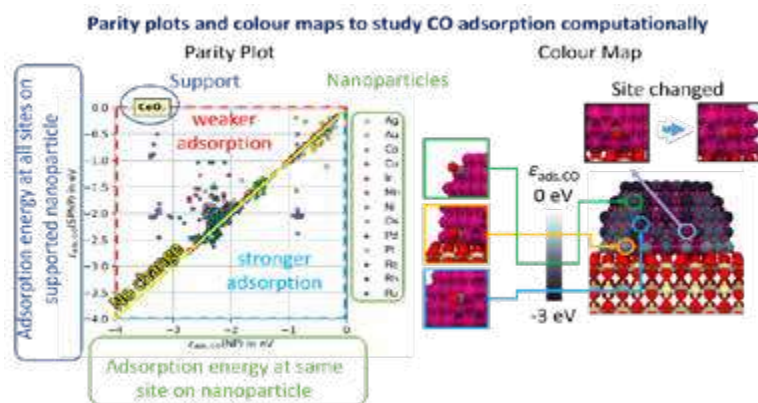
^aShinshu University.

*Corresponding author: valadez@shinshu-u.ac.jp, koyama_michihisa@shinshu-u.ac.jp

Abstract

More than 80% of industrial processes involve a catalytic step, with heterogeneous catalysis being particularly widespread. Metal nanoparticles supported on metal oxides serve as key catalysts for practical applications. Their performance, determined by stability, catalytic activity, and selectivity, may be influenced by metal-support interactions. However, fully understanding the factors contributing to the support effect remains a challenge. Density Functional Theory (DFT) studies have provided valuable insights into supported nanoparticle systems. Yet, as complexity increases, DFT calculations become impractical due to computational limitations. Neural Network Potentials have proven to be effective alternatives, successfully describing strong metal-support interactions that induce nanoparticle decoration¹. In this contribution, we use the PreFerred Potential (PFP)² to model CO adsorption on various supported nanoparticles. To handle extensive datasets, the support effect is analyzed through parity plots comparing supported nanoparticles with their vacuum counterparts, alongside color maps visualizing CO adsorption properties across different adsorption sites. The figure below illustrates this approach. Since CO activation is a crucial step in Fischer-Tropsch synthesis for liquid hydrocarbons, our results offer valuable insights into catalytic performance.

Keywords: Heterogeneous Catalysis, Neural Network Potential, Supported Nanoparticles, Metal-Support Interactions, CO Adsorption



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OBELiX: A CURATED DATASET OF CRYSTAL STRUCTURES AND EXPERIMENTALLY MEASURED IONIC CONDUCTIVITIES FOR LITHIUM SOLID-STATE ELECTROLYTES

Homin Shin^{a,*}, Félix Therrien^{b,*}, Jamal Abou Haibeh^{b,c}, Divya Sharma^b, Rhiannon Hendley^{a,d}, Alex Hernandez-Garcia^{b,e}, Sun Sun^a, Alain Tchagang^a, Jiang Su^a, Samuel Huberman^c, Yoshua Bengio^b, Hongyu Guo^{a,*}

^a National Research Council Canada, Ottawa, Canada

^b Mila, Montréal, Canada

^c Department of Chemical Engineering, McGill University, Montréal, Canada

^d Department of Chemistry and Biomolecular Science, University of Ottawa, Ottawa, Canada

^e Département d'informatique et de recherche opérationnelle, Université de Montréal, Montréal, Canada

*Corresponding author: homin.shin@nrc-cnrc.gc.ca; felix.therrien@mila.quebec; hongyu.guo@uottawa.ca

Abstract

Recently, a wide range of machine learning (ML) models including graph neural networks (GNNs) are being rapidly developed for materials science application. However, data scarcity, in particular, property-labelled data, hinders the application of such ML models in extracting the relationships between structures and materials properties. For example, Materials Project (MP) contains 144,595 inorganic materials, but only 76,240 electronic band structures, 14,072 elastic tensors, and 3402 piezoelectric tensors. Solid-state electrolyte batteries are expected to replace liquid electrolyte lithium-ion batteries in the near future thanks to their higher theoretical energy density and improved safety, for which relevant experimental ionic conductivity and structural datasets are very limited. Here, we present OBELiX, a domain-expert-curated database of 600 synthesized solid electrolyte materials and their experimentally measured room temperature ionic conductivities gathered from literature. Each material is described by their measured composition, space group and lattice parameters. A full-crystal description in the form of a crystallographic information file (CIF) is provided for 320 structures for which atomic positions were available. We discuss various statistics and features of the dataset and provide training and testing splits that avoid data leakage. Finally, we benchmark seven existing ML models on the task of predicting ionic conductivity and discuss their performance. The goal of this work is to facilitate the use of machine learning for solid-state electrolyte materials discovery.

Keywords: cheminformatics, solid-state, electrolytes, ionic conductivity, energy storage

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SMART FUEL QUALITY ASSURANCE THROUGH FOURIER TRANSFORM NEAR INFRARED (FTNIR) CHEMOMETRIC TECHNOLOGY

Anita Binti Jefrydin*, Irwan Tarmizi Talib, Sayed Omar Tn Sayed, Shafik Othman

*Corresponding author: anita_j@petronas.com

Abstract

Traditional laboratory-based analyses are time-consuming, prone to systematic errors, and reactive, often delaying decision-making for process optimization and product quality correction. This study highlights the application of Fourier Transform Near-Infrared (FTNIR) spectroscopy integrated with multivariate chemometric modeling as powerful digital tool for quality monitoring.

By leveraging Partial Least Square (PLS) regression and Principal Component Analysis (PCA), FTNIR enables simultaneous, non-destructive prediction of Research Octane Number (RON), distillation boiling points, and benzene concentrations in gasoline blending and certification. This FTNIR technology reduces product quality give away with tighter control of product specification allows rapid adaptation to blending adjustments. The chemometric models are calibrated and validated against certified laboratory prime test methods, achieving high prediction accuracy within minutes.

The adaptation of FTNIR technology enhances operational efficiency, reduces off-spec production and rebinding events, reduces laboratory operating cost, and supports data-driven decision making. This FTNIR technology not only improves product compliance with stringent fuel quality standards but also strengthens predictive capabilities for future smart refinery initiatives.

Keywords: FTNIR, chemometric, multivariate, PLS, PCA

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INTERPRETABLE INFRARED SPECTRA PREDICTION MODELS BASED ON STRUCTURAL NEIGHBORING MECHANISM

Chengchun Liu^a, Ruqiang Zou^{a,b}, Fanyang Mo^{a,b,c*}

^a*School of Materials Science and Engineering, Peking University, No.5 Yiheyuan Road, Haidian District, Beijing, 100871.*

^b*School of Advanced Materials, Peking University Shenzhen Graduate School, No.2199 Lishui Road, Nanshan District, Shenzhen, 518055.*

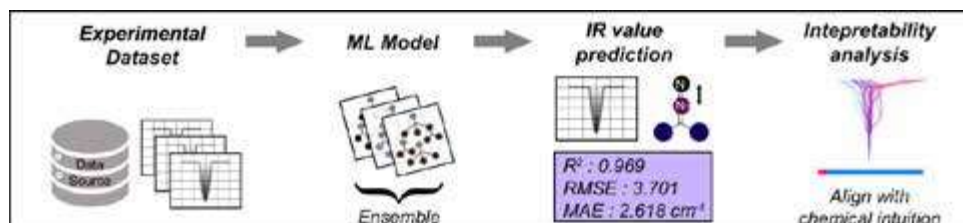
^c*Guangdong Provincial Key Laboratory of Nano-Micro Materials Research, Peking University Shenzhen Graduate School, No.2199 Lishui Road, Nanshan District, Shenzhen, 518055.*

*Corresponding author: fmo@pku.edu.cn

Abstract

Infrared (IR) spectroscopy is crucial for the study of molecular dynamics, offering real-time monitoring of chemical reactions. This not only reveals the microscopic mechanisms and kinetic features of reactions but also enables real-time dynamic monitoring of chemical synthesis components and supports a deeper understanding of molecular properties. A significant advantage of machine learning (ML) algorithms is their ability to identify complex correlations within large datasets, thus constructing models that predict previously unknown outcomes. Currently, predictions and analyses of infrared spectroscopy primarily rely on theoretical calculations and comparisons with existing spectral libraries. Therefore, developing infrared spectroscopy prediction models that combine high accuracy with strong generalizability is of great significance for scientific research. Data-driven based on knowledge embedding helps the algorithm to capture the rules between molecular structure and properties in large amounts of data, thereby improving the model's performance. Due to the unique vibrational and rotational modes of complex molecular fingerprints, predicting and analyzing infrared spectroscopy remains challenging. To this end, we have designed a knowledge embedding method based on the Structural Neighboring Mechanism (SNM), achieving the prediction of characteristic absorption frequencies in the infrared spectroscopy functional group region¹. Empirical evidence indicates that the infrared absorption values of functional groups are mainly influenced by adjacent atoms and bonds. Inspired by this, we propose a machine learning method that employs a structural neighboring mechanism, identifying key structural fragments near functional groups. By quantifying the types and values of chemical information, this method significantly enhances the predictive performance and interpretability of the infrared spectroscopy model. This approach not only reveals the close correlation between infrared spectroscopic features and molecular structure but also provides a scalable and efficient new paradigm for analyzing complex molecular interactions and their molecular fine structures' impact on infrared signals.

Keywords: infrared spectroscopy; knowledge embedding; interpretable machine learning



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MULTIMODAL LEARNING IN SYNTHETIC CHEMISTRY APPLICATIONS: GAS CHROMATOGRAPHY RETENTION TIME PREDICTION AND ISOMER SEPARATION OPTIMIZATION

Jinglong Lin^a, Longyin Song^b, Shufeng Chen^{b*}, Fanyang Mo^{a*},

^a*School of Materials Science and Engineering, Peking University*

^b*School of Chemistry and Chemical Engineering, Inner Mongolia University*

*Corresponding author: shufengchen@imu.edu.cn; fmo@pku.edu.cn

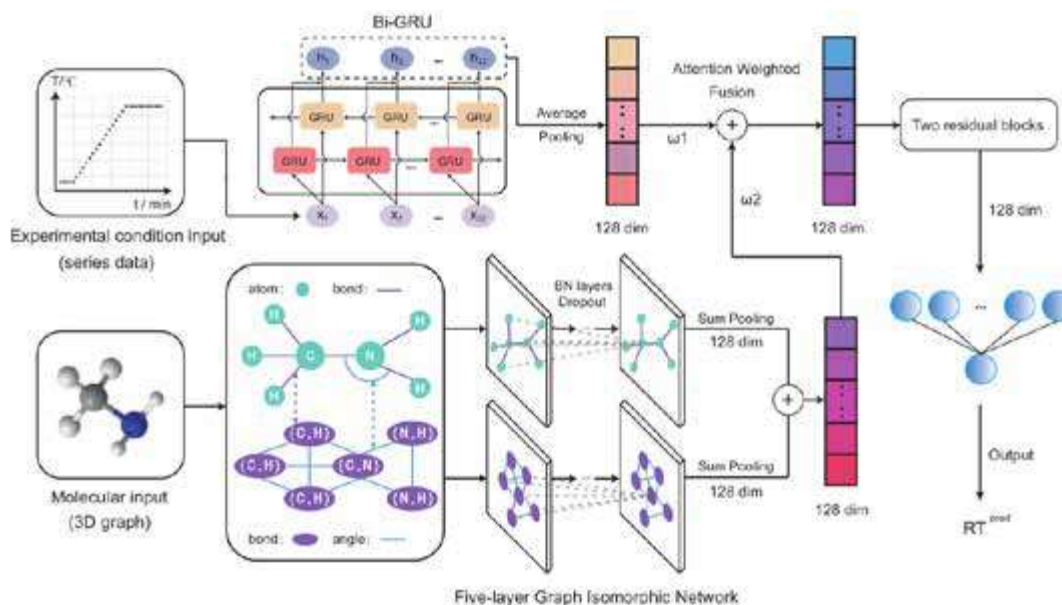
Abstract

Multimodal learning, a powerful machine learning (ML) technique, remains underexplored in chemistry. We propose an innovative multimodal framework for Gas Chromatography (GC) that combines a geometry-enhanced graph isomorphism network and gated recurrent units (GRU) to predict GC retention time (GC-RT) across various molecular heating profiles. The model achieves a test set R^2 of 0.995, outperforming traditional ML methods, and optimizes chromatographic conditions for separating positional and *cis/trans* isomers, reducing the need for experimental iterations.

Key contributions include:

1. Creation of a Gas Chromatography Retention Time (GCRT) dataset comprising 250 compounds and 3950 data points, and the development of the GC-PIEA method for batch extraction from chromatograms.
2. Construction of conventional ML models for GC-RT prediction and feature analysis.
3. Development of a multimodal model combining graph isomorphism and Bidirectional GRU, achieving R^2 of 0.995 with robust generalization capabilities.
4. Introduction of the isomer separation degree for virtual screening and the identification of optimal temperature programs.
5. A strategy using GC-RI and temperature programs for GC-RT prediction, with a pre-trained ANN model for broader RT prediction.

Keywords: gas chromatography, multimodal learning, retention time prediction, isomer separation



DEEPMASS: UNKNOWN COMPOUND ANNOTATION USING SEMANTIC MASS SPECTRAL SIMILARITY AND CHEMICAL SPACE LOCALIZATION

Hongchao Ji^{a,*}

^a*Agricultural Genomics Institute at Shenzhen, Chinese Academy of Agricultural Sciences, Shenzhen, 518120, China PR.*

**Corresponding author: jihongchao@caas.cn*

Abstract

Untargeted analysis using liquid chromatography-mass spectrometry (LC-MS) enables the quantification of both known and unknown compounds within biological systems. However, in practical applications, the majority of compounds often remain unidentified due to the complexity of biological matrices. In this work, we present DeepMASS v2^{1,2}, an advanced deep learning-based method designed to enhance the annotation of metabolites by leveraging mass spectral semantic similarity analysis and chemical space localization for improved structural prediction of unknown compounds. Addressing the challenge of “chemical dark matter” in untargeted LC-MS analysis—where a large portion of compounds remain unidentified due to limited reference libraries—DeepMASS v2 utilizes an unsupervised Word2Vec model to embed mass spectra into semantic vectors. These vectors, in combination with Hierarchical Navigable Small World (HNSW) graph-based search algorithms, allow for efficient identification of structurally analogous “neighbor compounds” from reference databases. Furthermore, Morgan fingerprint-guided chemical space localization refines candidate ranking by contextualizing structural relationships. Experimental validation using CASMI and natural product benchmark datasets demonstrated superior performance, with Top-1 accuracy rates of 57.7% and 47.4%, respectively—outperforming existing tools like SIRIUS and MS-Finder. Notably, DeepMASS v2 also excelled in annotating compounds absent from reference libraries, achieving a 33.7% Top-1 accuracy in this context. A case study on tomato ripening metabolomics further highlighted the tool’s capabilities, annotating over 93% of metabolic features and uncovering dynamic changes in metabolites related to flavor and resistance.

Keywords: Untargeted LC-MS; Mass spectral annotation; Chemical space localization; Semantic similarity

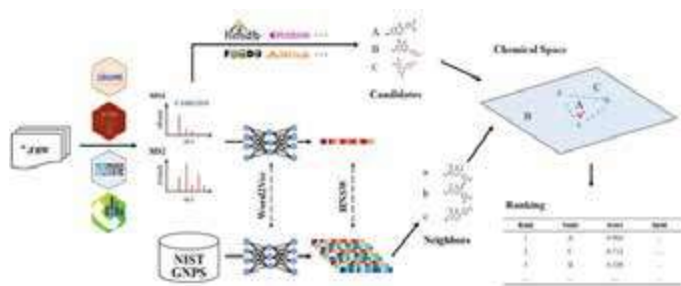


Fig. 1. Workflow of DeepMASS. Raw mass spectrometry data are preprocessed, and unannotated compound signals are parsed into MS1 and MS2 spectral data. MS1 is used to predict the molecular formula, which is then leveraged to retrieve candidate structures from chemical libraries. MS2 spectra are embedded and used to search for structurally similar neighbors through a semantic embedding model trained on existing spectral databases. Both candidate and reference structures are projected into chemical space based on chemical fingerprints. The correct structure of the unknown compound is determined by evaluating the relative positions of the candidate and reference structures within the chemical space.

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EVALUATION OF THE THERAPEUTIC POTENTIAL OF A NOVEL CURCUMIN ANALOGS FOR DRUG-RESISTANT HEAD AND NECK SQUAMOUS CARCINOMA BY TARGETING PLA2/TREM2/TNC SIGNALING HUB

Nur Azizah^{1,2}, Ritmaleni^{2,*}, Rumiya^{2,*}, Alexander T.H Wu^{3,*}

¹Master in Pharmaceutical Sciences, Faculty of Pharmacy, Gadjah Mada University, Indonesia.

²Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Gadjah Mada University, Indonesia

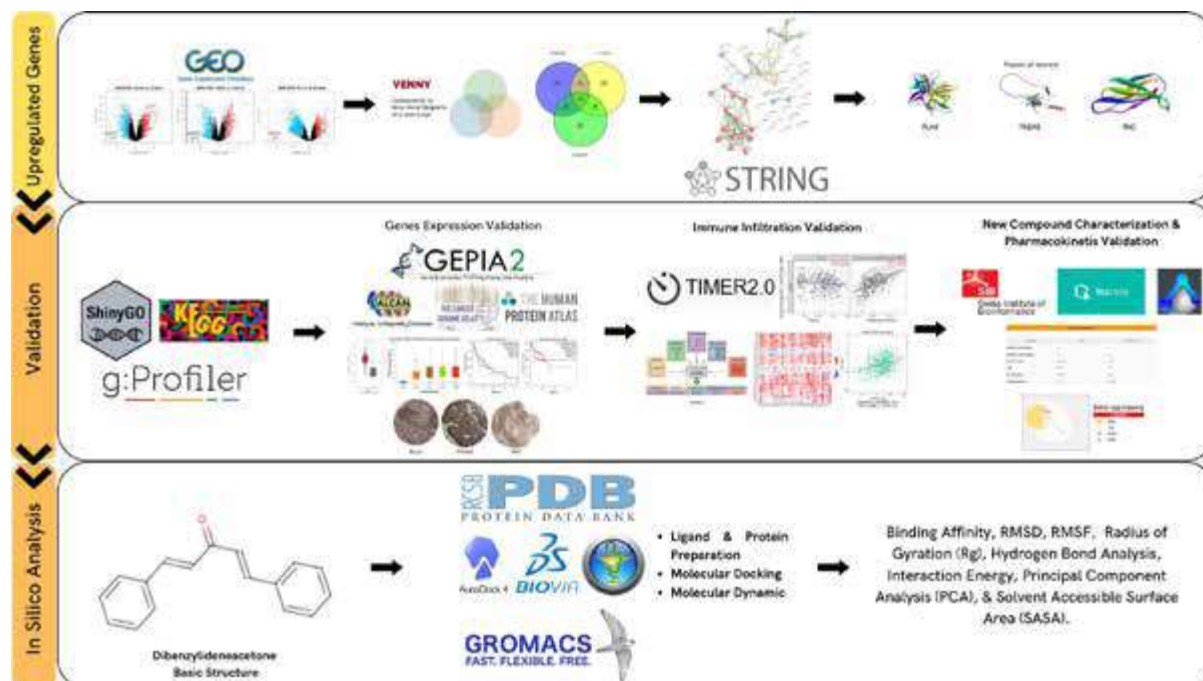
³The Ph.D. Program of Translational Medicine, College of Medical Science and Technology, Taipei Medical University, Taiwan

*Corresponding author: ritmaleni@ugm.ac.id; rumiyaris@ugm.ac.id; chaw1211@tmu.edu.tw

Abstract

HNSCC frequently detected at advanced stages due to a lack of cancer awareness, socioeconomic problem, and dependence on alternative medicine often lead to late-stage HNSCC diagnosis. This reduces treatment results and survival. In Indonesia, HNSCC is a serious public health issue with varying incidence and characteristics, and it is expected that HNSCC will rise by 30% by 2030. This study examined the effectiveness of curcumin analogs in the treatment of HNSCC. We relied on the inhibition of proteins PLA2, TREM2, and TNC. We analyzed various GEO databases to identify upregulated genes, evaluating gene expression and immune infiltration. We performed molecular docking of Dibenzylideneacetone (DBA) group as curcumin analogs complex with PLA2, TREM2, and TNC to validate. Our study revealed that the PLA2, TREM2, and TNC were highly expressed in HNSCC tissues compared to adjacent normal tissues. Increased levels of these proteins are significantly associated with inflammation, mainly through immune-mediated expression. The molecular docking data indicated good binding affinities compared to the standard therapy. In conclusion, our study identified the expression of upregulated gene signatures PLA2, TREM2, and TNC associated with HNSCC, immune infiltration profiles, and potential drug candidates for HNSCC, highlighting the effectiveness of DBA inhibiting the inflammatory pathway. For the next step, we will focus on molecular dynamics to collect further data for this research.

Keywords: HNSCC; DBA; Curcumin Analogs; PLA2/TREM2/TNC; Molecular Docking



INTEGRATING MACHINE LEARNING AND IN SILICO APPROACHES TO IDENTIFY NOVEL INNEXIN-2 HEMICHANNEL INHIBITORS FOR ANTIPARASITIC DRUG DEVELOPMENT

Sbarbaro Christopher^a, Seron Nicolás^a, Loncón Macarena^a, Márquez Valeria^a, Duarte Yorley^{a*}.

^aCenter for Bioinformatics and Integrative Biology, Facultad de Ciencias de la Vida, Universidad Andrés Bello, Av. República 330, Santiago 8370146, Chile

*Corresponding author: yorley.duarte@unab.cl

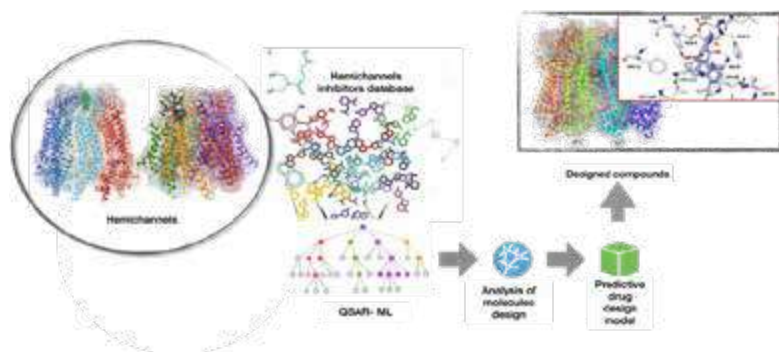
Abstract

Gap junctions are specialized intercellular channels essential for direct communication between adjacent cells, allowing the transfer of small molecules and ions critical for cellular coordination. In invertebrates, this role is fulfilled by innexins (Inxs), with Innexin-2 (Inx2) being particularly vital for maintaining intercellular signaling across tissues.¹ Targeting Inx hemichannels represents a promising strategy for developing next generation antiparasitic agents. The parasitic sea louse *Caligus rogercresceyi*, a significant threat to the Chilean salmon farming industry, demonstrates increasing resistance to traditional treatments, prompting the need for novel molecular targets. Despite the presence of innexin hemichannels in *Caligus*, their pharmacological regulation remains poorly understood.²

In this study, we applied a combined in silico and machine learning (ML) approach to identify and evaluate potential Inx2 inhibitors. Despite limited specificity for innexin subtypes, a curated dataset of approximately 50 hemichannel modulators was assembled, incorporating known inhibitors and novel molecules synthesized and tested by our group. This dataset was used to train ML-QSAR models utilizing various molecular descriptors and fingerprints. Different ML models were generated, each optimized to predict inhibitory activity. Compounds showing high predictive alignment were selected, and the top 10 underwent further in silico evaluation, with 5 prioritized for future synthesis and experimental validation. Parallel to the QSAR modeling, we developed a high-confidence structural model of the *Caligus* Inx2 hemichannel using AlphaFold2 and predicted binding pockets. Molecular docking and dynamics simulations revealed stable interactions and significant alterations in electrostatic surface potential, suggesting permeability-based inhibition mechanisms.

These findings provide a foundation for rational Inx2 inhibitor design and highlight the potential of integrative ML and structural biology strategies in antiparasitic drug discovery.

Keywords: Innexin, Molecular docking, machine learning, Molecular Dynamics



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AN INTEGRATED STRATEGY OF UHPLC-ESI-MS/MS COMBINED WITH BIOACTIVITY-BASED MOLECULAR NETWORKING FOR IDENTIFICATION OF DENGUE ACTIVITY FROM *BRUCEA JAVANICA* (L.) MERR

Nor Syaidatul Akmal Mohd Yousof^{a,b,*}, Mohd Ridzuan Mohd Abdul Razak^a,
Nor Hadiani Ismail^b

^aHerbal Medicine Research Centre, Institute for Medical Research, National Institutes of Health, Ministry of Health, No. 1 Jalan Setia Murni U13/52, Seksyen U13, Setia Alam, 40170 Shah Alam, Selangor Darul Ehsan, Malaysia.

^bFaculty of Applied Science, UiTM, 40450 Shah Alam, Selangor, Malaysia.

*Corresponding author: syaidatul.akmal@moh.gov.my

Abstract

Brucea javanica, a Malaysian native species from Simaroubaceae family, is a promising source of bioactive compounds, particularly quassinoids and tryptophan alkaloids, known for their antiviral properties. This study aimed to streamline the discovery of bioactive compounds by dereplicating the extract and partitions of *B. javanica* root. Ultra-high-performance liquid chromatography tandem mass spectrometry (UHPLC-MS/MS) was used to analyse the extract, and the resulting mass spectrometry data were processed through the GNPS platform to generate molecular networking. The molecular networking and *in silico* structural annotation of 345 *m/z* features, identified potentially bioactive compounds, particularly in fractions F4–F9. Bioactivity-based molecular networking highlighted the significant antiviral activity of tryptophan alkaloids, with a bioactivity score of $r \geq 0.85$ and $p\text{-value} \leq 0.05$. In contrast, quassinoids exhibited only a weak correlation with anti-dengue activity. Targeting the tryptophan alkaloids, particularly canthin-6-one derivatives, may provide a promising direction for antiviral drug development. The EC_{50} values of the isolated compounds (canthin-6-one **1**, 5-methoxycanthin-6-one **2**, canthin-6-one N-oxide **3**, 1-hydroxy-11-methoxycanthin-6-one **4**, and bruceoline J **5** and E **6**) ranged from 0.86 to 6.1 $\mu\text{g/mL}$, with SI values between 1.85 and 63. These findings underscore the therapeutic potential of canthin-6-one derivatives and highlight the need for further mechanistic and *in vivo* studies to validate their efficacy against dengue virus.

Keywords: Melada pahit, dengue, bioactivity molecular networking

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PRELIMINARY IN SILICO STUDIES OF PHYTOCHEMICALS FROM SELECTED HERBAL PLANTS AS POTENTIAL JAPANESE ENCEPHALITIS VIRUS INHIBITOR

Afiq Azil^{a,*}, Kirubagari R. Kumar^a, Nur Hidayah Saiful Bahari^a

^aSchool of Pharmacy, KPJ Healthcare University.

*Corresponding author: ucn.afiqazil@kpju.edu.my

Abstract

Japanese encephalitis virus (JEV), spread by *Culex* mosquitoes, causes viral encephalitis in many Asian countries. While vaccination offers prevention, its effectiveness diminishes over time and can cause mild side effects. Therefore, a targeted therapeutic agent is needed to cure JEV infection. The purpose of this study was to evaluate the inhibitory potential of phytochemicals from three herbal plants namely *Eurycoma longifolia* (Tongkat Ali), *Peuraria montana* (Kudzu), and *Piper betle* (Sirih) against JEV envelope (E) protein. The phytochemicals were subjected to in silico pharmacokinetics assessment; adsorption, distribution, metabolism, excretion, toxicity (ADMET) as well as molecular docking simulation with the E protein. Three compounds from each plant that exhibits the greatest potential in the ADMET screening and fulfilling Veber, Lipinski, Ghose and Muegge criterias for drug-likeness were successfully docked against the E protein. Eurycolactone C from *Eurycoma longifolia* showed the highest binding affinity ($-6.7 \text{ kcalmol}^{-1}$) followed by irisolidine ($-6.2 \text{ kcalmol}^{-1}$) from *Peuraria Montana* and emodin ($-5.9 \text{ kcalmol}^{-1}$) from *Piper Betle*. Further protein ligand interaction analysis confirmed the interaction stability of the Eurycolactone C with E protein is supported by having multiple hydrogen bond, hydrophobic interaction and a salt bridge interaction. The findings revealed that specifically Eurycolactone C has traits that make it a suitable candidate to be used as lead compound in the development of novel therapeutics and strengthen *Eurycoma longifolia* potential as a herbal plant. Its substantial interaction with the E protein can be utilized for further investigation in developing potential antiviral medication against JEV.

Keywords: ADMET; molecular docking; Japanese Encephalitis; virus inhibitor; herbal plants



PLATFORMS FOR AUTOMATED STORAGE AND ANALYSIS OF CHEMICAL DATA

Philippe Gantzer*, Yuuya Nagata, Pavel Sidorov

Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Japan.

**Corresponding author: p.gantzer@icredd.hokudai.ac.jp*

Abstract

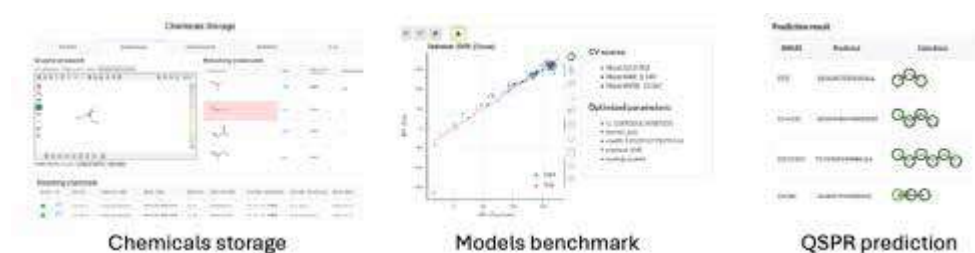
The digitalization of data and adoption of robotics are becoming an important step towards the automation of chemical laboratories.¹ Notably, the development of informatics tools for the automated management and analysis of experimental data is an integral part of this task. However, their implementation is often challenging and requires a strong collaboration between chemists and informaticians. The Institute for Chemical Reaction Design and Discovery (WPI-ICReDD) has been created to tackle challenges related to the design and discovery of new chemical reactions by fusing different fields of chemistry (experimental, computational and informatics). In this poster, we would like to introduce some of the tools we have created to aid and collaborate with experimental chemists.

CGRdb2.0² is a Python open-source database system developed by our team, specifically designed for storing and searching molecules, reactions, and associated chemical data. Two databases with user-friendly web interfaces have been derived from CGRdb2.0. StockDB monitors and searches compounds within the labs' chemical stock, providing various information such as chemicals locations, manufacturer, purchasing date, quantities, CAS numbers and SMILES. CatalystDB is an extension to StockDB that stores organic catalysts synthesized in-house by the List Platform (Hokkaido University) and can perform partial searches by R groups.

DOPTools³ is a Python open-source library we designed to create QSPR predictive models and conduct benchmarks over different descriptor types and modeling algorithms seamlessly. We initially released a command-line interface (CLI) allowing a full exploitation of its features but requiring coding experience. We subsequently developed a web-based graphical user interface (GUI) version using the CADS platform,⁴ allowing users to easily progress from data management to predictive modeling.

The examples presented on this poster highlight our initial efforts in developing tools to support collaborative research between researchers of different chemistry fields and support the automatization of chemical laboratories.

Keywords: chemical automation, machine learning, chemical databases



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MACHINE LEARNING-BASED PREDICTION OF COMPOUND AQUEOUS SOLUBILITY USING MOLECULAR DESCRIPTORS AND FINGERPRINTS

Teo Chian Ying^{a,*}, Wong Zi Yang^a, Pravina A/P Ellambarathi^a, Fong Pui Kwan^b

^aDepartment of Pharmaceutical Chemistry, School of Pharmacy, IMU University, 57000 Kuala Lumpur, Malaysia.

^bCentre for Digital Health & Health Informatics, School of Business and Technology, IMU University, 57000 Kuala Lumpur, Malaysia.

*Corresponding author: TeoChianYing@imu.edu.my

Abstract

Accurate prediction of aqueous solubility is crucial for sustainable drug discovery and development. In this study, machine learning techniques were applied to model and predict the solubility of chemical compounds using the AqSolDB dataset. Molecular descriptors and fingerprints were computed to represent the structural and physicochemical properties of compounds. The dataset was divided into training and testing sets, with five-fold cross-validation employed for model evaluation. Three models—Multiple Linear Regression (MLR), Random Forest (RF), and Light Gradient Boosting Machine (LightGBM)—were trained and further fine-tuned to optimize different hyperparameters. Model performance was assessed using evaluation metrics, including coefficient of determination (R^2), mean absolute error (MAE), and root mean squared error (RMSE). Tree-based models (RF and LightGBM) outperformed MLR, demonstrating better predictive accuracy. To enhance interpretability, SHapley Additive exPlanations (SHAP) were utilized to analyze the contribution of individual molecular descriptors and fingerprints to solubility predictions. The analysis revealed key molecular features influencing solubility, providing insights into the underlying chemical factors. These findings underscore the potential of combining advanced machine learning techniques with molecular representations to achieve accurate and interpretable predictions of compound solubility.

Keywords: machine learning, aqueous solubility, prediction, molecular descriptors, molecular fingerprints

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NANOENGINEERING ANTIMICROBIAL MACROMOLECULES VIA THE AMINE UNCAGING STRATEGY

Edgar H. H. Wong^{a,*}, Zeyu Shao^a, Hao Luo^a

^a*School of Chemical Engineering, University of New South Wales, Sydney, NSW 2052, Australia.*

**Corresponding author: edgar.wong@unsw.edu.au*

Abstract

The increasing number of infections caused by multidrug-resistant bacteria is now considered a critical global healthcare issue.¹ To overcome this, antimicrobial peptides (AMPs) and mimics thereof have emerged as promising candidates as potential new antimicrobial drugs given their ability to kill bacteria with minimal resistance development.^{2,3,4} Unlike traditional antibiotics that act on intracellular targets, this class of compounds, which contain cationic (amines) and hydrophobic groups, exert their activity by perturbing the bacteria cell membrane, thereby making it harder for the bacteria to resist and develop resistance. However, this class of compounds also tend to exhibit toxicity toward mammalian cells (and thus poor selectivity), hence hindering their application in clinical settings. The main reason for this poor selectivity is due to the non-specific interaction/binding between the cationic groups of the antimicrobial agent with cell membranes.

To overcome this selectivity issue, our group have been developing novel AMP mimics wherein the cationic amines are initially masked/caged like a prodrug (hence benign and safe) but can be activated/uncaged using specific triggers to confer on-demand antimicrobial activity. This approach, termed as the amine uncaging strategy (AUS), focusses on addressing the root cause of toxicity (i.e., the cationic amine groups) to improve biocompatibility whilst enabling for the precise activation of antimicrobial activity through strategic uncaging chemistries. Thus far, we have developed several systems based on external (photo),⁵ bio (enzymes),^{6,7} and chemical (click) activations to highlight the benefits of AUS in antimicrobial drug design.

Keywords: antimicrobial peptides, prodrugs, multidrug-resistant bacteria, stimuli-responsive, self-assembly

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“POLLUTED MICROENVIRONMENT AND HEALTH”

Asmita Patil^{1*}, Swarnabha Sarkar¹, Aditya Dontham¹, Revand Ravindran¹, Abhishek Kandpal²,

Debabrata Dasgupta², Bahni Ray², Mayank Kumar²

Department of Physiology, All India Institute of Medical Sciences, New Delhi

Department of Mechanical Engineering, Indian Institute of Technology, New Delhi

**Corresponding author: drasmita@aiims.edu*

Abstract

Air pollution is a major deterrent to health throughout the world, especially in the developing countries. Researchers have demonstrated the role of particulate component of Diesel exhaust affecting health. The addition of filters in automobiles and air purifiers at home and workplace and personal use of N-95 masks to a much larger extent, helps to protect from the particulate fraction of pollutants. However, the gaseous fraction remains majorly unavoidable, generating a risk for developing stroke, ischaemic heart disease, chronic obstructive pulmonary disease, and infertility. Population based studies have linked pollution to increased incidence of adverse pregnancy outcomes.

Our group has performed studies in male wistar rats, in an indigenous self-fabricated whole body exposure chamber to investigate the effect of the filtered fraction of diesel exhaust (predominantly comprising gases) on the regulatory mechanisms of the male reproductive function by assessing sperm parameters, histopathology of testis, levels of principal hormones of HPG axis along with concentrations of xenobiotic agent specific anti-oxidant enzyme (GST) that govern the homeostatic regulation of testicular milieu in adult male Wistar rats. We are also studying the effect of pollution on cardiovascular protective mechanisms. And the role of Vitamin C and E as putative antioxidants for protection from air pollution. Our research focuses on the chemical composition of filtered diesel exhaust and its association with bio-molecular mechanisms underlying the pathogenesis of Diesel exhaust induced diseases.

The objective was to develop a WBE unit to study the effect of diesel engine exhaust on male reproductive function by focusing on the following specific objectives:

1. Fabrication and development of exposure unit
2. Study the effect of diesel exhaust exposure through the WBE unit on fertility
3. Study the effect of diesel exhaust exposure through the WBE unit on cardiovascular reflex

Keywords: Microenvironment, Diesel Exhaust, Reproductive Health, Wistar Rats

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ANALYSIS OF TERPENE PROFILES AND THE MOSQUITO LARVICIDAL ACTIVITY OF THE ESSENTIAL OILS OF A MEDICINAL *CANNABIS SATIVA* L. CULTIVAR

Ronnie Blair^a, Roy Porter^{a*}, Simone Sandiford^a

^aUniversity of the West Indies, Mona, Jamaica

*Corresponding author: roy.porter@uwimona.edu.jm

Abstract

Cannabis is one of the little known multi-billion-dollar plants where scientific information relating to its chemical and genetic diversity is unknown. With its growing legalization, there is more of an interest in a science-based classification system. The current “vernacular” classification system is unregulated and studies have shown that this system is arbitrary and does not reflect any specific, unique genotype or chemotype.¹ Terpenes are secondary metabolites in cannabis that contribute to the overall effect of cannabis variety. Unique terpene chemical fingerprints have successfully been used to distinguish amongst cannabis varieties.²

Post-harvest processes such as drying and curing are crucial in product development and directly affects the quality, therapeutic activity and shelf-life of cannabis cultivars.³ Few studies have examined the effect of such processes on cannabis products. This study aims to assess the terpene profiles and the mosquito larvicidal activity of a medicinal *Cannabis sativa* L cultivar throughout flowering and post-harvest processes.

Essential oils were extracted via Hydro distillation and subsequently analyzed by Gas Chromatography Flame Ionization detector (GC-FID) and Gas Chromatography–Mass spectrometry (GC–MS). A total of 34 compounds were identified with the abundant terpenes being terpinolene, beta-myrcene and beta-ocimene. The essential oils also exhibited larvicidal activity against *Aedes aegypti* mosquito larvae with an LC₅₀ value of 95.46 µg/ml.

Keywords: natural products, Cannabis sativa, essential oils, Aedes aegypti mosquito, larvicidal activity

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TICKS REPELLENTS: A PERSPECTIVE FOR THE CREATION OF A CONTROL RELEASE MATERIALS

Sergey Andreev^{a,*}, Andrey Kuzovlev^{a,b}, Alisa Terskova^a, Konstantin Sakharov^c,

^a *Disinfectology Institute of F.F. Erisman FSCH of Rospotrebnadzor, Moscow, Russia*

^b *The Institute of Environmental and Agricultural Biology (X-BIO), University of Tyumen, Tyumen, Russia*

^c *School of Materials Science and Engineering, Nanyang Technological University, Republic of Singapore*

*Corresponding author: svandreev.niid@gmail.com

Abstract

Vector-borne diseases account for more than 17% of all infectious diseases, causing more than 700 000 deaths annually ¹. Ticks are one of the major vectors of many dangerous diseases. The objective of this study is to develop materials that possess repellent properties against ticks. All materials were tested in a natural habitat, focusing on the most epidemiologically significant tick species in Russia: the taiga tick.

The main points of this work:

1. Textiles based on permethrin and cypermethrin are effective in preventing tick bites. Polymer films containing pyrethroids are formatted onto the surface of the fabric and provide a long-lasting effect ².
2. Synthetic and natural repellents are effective against taiga tick. DEET and IR3535 are the most effective ³. It seems that the contact action is the preliminary mechanism for repellency.
3. Polymer composites containing repellents are promising for tick bite prevention with controlled release. Thermal diffusion activated by currency or heat could be used for release activation⁴electrically conductive polymer composites based on repellent N,N-diethyl-3-methylbenzamide with concentrations ranging from 6 to 30 wt% were developed. The electrical resistivity of repellent composites, as determined by electrochemical impedance spectra, ranges from 150 to 171 Ohm, which allows such materials to be used when a low voltage is applied. The study of the rheological properties of the obtained repellent composites and the analysis of the TGA curves demonstrated that the dynamic viscosity of the materials has a significant effect on the thermal diffusion of the repellent. The study of the thermal diffusion of N,N-diethyl-3-methylbenzamide demonstrated that a higher yield of repellent (up to 36.4×10^{-8} mol).

As a result, we have developed clothing to protect against ticks. We have also developed a new platform to control the release of tick repellents. All materials were effective in a field trial.

Keywords: repellents, control release, smart textile, ticks, infectious diseases

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ANTIVIRAL POTENTIAL OF *EUPHORBIA* SPP. EXTRACTS AGAINST SARS-COV-2 AND DENGUE VIRUS TYPE-2

Maizatul Hasyima Omar^{a*}, Amirrudin Muhammad^b, Noorsofiana Padlan^b, Nur Hannani Ahmad Rozani^a, Mohd Ridzuan Mohd Abd Razak^b

^aPhytochemistry Unit, Herbal Medicine Research Centre, Institute for Medical Research, National Institutes of Health, Setia Alam 40170 Shah Alam Selangor;

^bBioassay Unit, Herbal Medicine Research Centre, Institute for Medical Research, National Institutes of Health, Setia Alam 40170 Shah Alam Selangor;

*Corresponding author: maizatul.hasyima@moh.gov.my

Abstract

The Euphorbiaceae family has been widely utilized for its therapeutic properties, including antiviral, antimicrobial, antiulcer, antihypertensive, and muscle relaxant effects¹. Previous *in silico* studies have highlighted the potential of phytochemicals from *Euphorbia* species as inhibitors of SARS-CoV-2². However, experimental validation remains limited. This study aimed to assess the antiviral efficacy of extracts from selected *Euphorbia* species against SARS-CoV-2 and dengue virus serotype 2 (DENV-2). Extracts were prepared from *E. pulcherrima*, *E. pulmerioides*, *E. milli*, *E. trigona*, *E. geroldii*, *E. tirucalli*, and *E. hirta* collected from Malaysia. Antiviral activity was evaluated using a cytopathic effect (CPE) inhibition assay for SARS-CoV-2 and a plaque reduction assay for DENV-2. Several extracts showed potent inhibitory activities against both viruses, with EC₅₀ values for SARS-CoV-2 ranging from 2.7 to 50 µg/mL across various samples, all while maintaining cell viability. These findings provide supportive experimental data for the antiviral potential of *Euphorbia* species and lay the foundation for further studies to elucidate their active compounds and mechanisms of action.

Keywords: *Euphorbia* species, SARS-CoV-2, Dengue, CPE reduction assay, Plaque assay

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SOCIO-ENVIRONMENTAL DETERMINANTS OF *LEGIONELLA PNEUMOPHILA* IN DIVERSE WATER SYSTEMS: ANALYTICAL INSIGHTS AND RISK IMPLICATIONS

^aAtheesha Singh

^aWater and Health Research Centre, University of Johannesburg, Johannesburg, South Africa

*Corresponding author: asingh@uj.ac.za

Abstract

Legionella pneumophila poses a substantial public health challenge in regions with aging or insufficient water infrastructure—conditions common in many parts of South Africa^{1,2}. This study investigated *Legionella* contamination in water systems across urban (Hillbrow, Atteridgeville), informal (Zandspruit, Melusi), and rural (Vhembe) settings in South Africa from October 2022 to July 2024.

Samples from taps, geysers, storage tanks, and biofilms were analysed using Legiolert™, and PCR/qPCR methods. Significant disparities in *Legionella* contamination levels across the studied regions, correlated with variations in infrastructure age, plumbing system complexity, socio-economic conditions, water management practices, and environmental temperature fluctuations. The investigation revealed considerable variation in *Legionella* contamination across different socio-economic contexts. Contamination levels varied widely—from non-detectable to >2272.6 MPN/100 mL—with the highest concentrations found in high-density urban sites and rural locations with stagnant water. *Legionella* growth occurred across temperature ranges from 16.9°C to 49.1°C, confirming the adaptability of the pathogen across varied climatic conditions. Key drivers of *Legionella* proliferation included fluctuating water temperatures (16.9–49.1°C), plumbing materials (copper, PVC), and inadequate storage conditions. Informal settlements showed inconsistent patterns; Zandspruit, for example, exhibited elevated levels linked to poor container hygiene and intermittent supply.

Molecular methods outperformed culture-based approaches by detecting viable but non-culturable organisms. Legiolert™ offered rapid and specific detection, supporting its potential for routine surveillance in resource-limited settings.

Despite widespread environmental detection, clinical reporting remains low, potentially due to underdiagnosis, high HIV prevalence influencing host response, or limited diagnostic capacity^{3,4}. This study highlights critical relationships between socio-economic factors, infrastructure inadequacies, climatic conditions, and *Legionella* contamination in South Africa. This work emphasizes the need for integrated monitoring strategies, infrastructure renewal, and public health education to mitigate *Legionella*-associated risks in climate-sensitive and resource-constrained settings.

Keywords: Water infrastructure, Informal settlements, Geysers and storage tanks

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THE PROTECTIVE POTENTIAL OF CURCUMIN ANALOGS (PGV-5, HGV-5, THPGV-5, AND THHGV-5) ON UV A-INDUCED HUMAN DERMAL FIBROBLASTS

Rumiyati^{a*}, Ritmaleni^{b,c}, Eduardo Harya Satria P.^d, Hanisa Febrianti^d

^aLaboratory of Macromolecular Engineering, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Gadjah Mada University, Sekip Utara, Yogyakarta, Indonesia, 55281

^bCurcumin Research Center, Faculty of Pharmacy, Gadjah Mada University, Sekip Utara, Yogyakarta, Indonesia, 55281

^cLaboratory of Medicinal Chemistry, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Gadjah Mada University, Sekip Utara, Yogyakarta, Indonesia, 55281.

^dFaculty of Pharmacy, Gadjah Mada University, Sekip Utara, Yogyakarta, Indonesia. 55281..

*Corresponding author: rumiyaris@ugm.ac.id

Abstract

A high ultra violet A (UV A) exposure can harm skin and have negative impacts such as skin photoaging. The exposure can increase in intracellular reactive oxygen species (ROS) that cause wrinkles, a loss of skin tone, flexibility and skin cancer. These conditions may necessitate additional attention to the skin's health such as applying a cream to the skin. Researches to screen agents with protective effect of UV exposure are crucial undertaking. Some of the agents with the effects are curcumin and its analog. The purpose of this study is to assess potential of curcumin analogs against the intracellular ROS buildup caused by UV A in human dermal fibroblasts (HDF). Four curcumin analogs (PGV-5, HGV-5, THPGV-5, and THHGV-5) will be assessed in their skin-protective potential. Cell line cultures of HDFs were first treated with curcumin analogs at various concentrations for two hours, and then they were exposed to 3 J/cm² UVA radiation in order to investigate this effect. Cell viability was measured using the MTT assay. The measured effective concentration that can protect the cells was utilized for intracellular ROS investigation using the flow cytometry-DCFDA. It was demonstrated that there were cytoprotective effects of PGV-5, HGV-5, THPGV-5, and THHGV-5 on HDFs stimulated by 3 J/cm² UV A. Following the UV A irradiation, these compounds in the concentration range of 1–4 μM can keep HDF viability over 90%. HDFs can be shielded from the buildup of intracellular ROS by 1 μM the curcumin analogs. According to this finding, the curcumin analogs have a potential to protect the UV A exposure. Compared to the controls, the potency are higher than vitamin E and curcumin. Due to this potency, the curcumin analogs could be proposed as potential active components in cytoprotective agents especially to the UV A.

Keywords: protective effect, UV A, curcumin analog, Human Dermal Fibroblasts

UNIQUE PHYSICOCHEMICAL AND ANTIOXIDANT PROPERTIES DIFFERENTIATE STINGLESS BEE HONEY PRODUCED IN ACACIA FOREST FROM PENINSULAR AND BORNEO MALAYSIA

Ilya Dayini Azeman^a, Farah Adilah Md Jafray^b, Rabiatal Adawiah Mohd Noor^b,
Arif Zaidi Jusoh^c, Mohd Azerulazree Jamilan^d, Norhasnida Zawawi^{b*}

^aDepartment of Food Science, Faculty of Food Science and Technology, Universiti Putra Malaysia

^bLaboratory of Halal Services, Halal Products Research Institute, Universiti Putra Malaysia

^cFood Science and Technology Research Centre, Malaysian Agricultural Research and Development Institute (MARDI), Serdang, Malaysia

^dNutrition Unit, Nutrition, Metabolism and Cardiovascular Research Centre, Institute for Medical Research, National Institute of Health Malaysia

*Corresponding author: norhasnida@upm.edu.my

Abstract

Stingless bee honey (SBH), known for its bioactive compounds and nutraceutical properties, has been found to have homogenous quality when produced in Peninsular Malaysia (Mat Ramlan *et al.*, 2023). This study monitored the physicochemical properties and bioactive compounds of *Heterotrigona itama* honey from acacia forests in Selangor and Sarawak, Malaysia, and assessed its compliance with CODEX and Malaysian standards. Nine honey samples were analysed for moisture content, total soluble solids, pH, free acidity, color, electrical conductivity, and bioactive compounds, including sugars, organic acids, vitamins, phytochemicals, and antioxidants. To study their bioactive compounds, samples were analysed and quantified using HPLC-ELSD, HPLC-DAD, and LC-MS/MS. Statistical analysis included the Analysis of Variance (ANOVA), and Tukey's pairwise comparison ($P < 0.05$) was conducted using GraphPad Prism 10.3.0, while the Principal Component analysis (PCA) was performed using JMP Pro 17.1.0. The results showed that Sarawak honey had higher fructose, glucose, and trehalulose sugars and a higher moisture content. In contrast, Selangor honeys contain higher riboflavin, folic acid, total phenolic and flavonoid contents, which correlate with higher antioxidant properties, are darker and redder in color, and have better electrical conductivity, which correlates with the higher organic acid contents. Among organic acids, gluconic acid was predominant and higher in both samples. Rutin and chrysin, unique flavonoid markers, were found to differentiate Selangor and Sarawak's SBH, while PCA analysis was able to distinguish the samples further. The findings indicate that regional environmental factors influence SBH composition. This study provides valuable insights for differentiating SBH based on origin and guiding marketing strategies for regional products. Future research should explore broader sampling and evaluate health benefits to establish the uniqueness of SBH produced in Peninsular Malaysia and Borneo.

Keywords: antioxidants, phytochemicals, trehalulose, nutraceutical, phenolic compounds

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3D PRINTED BIOSPONGE ADSORBERS FOR CAPTURING TOXIC CHEMOTHERAPY DRUGS TO REDUCE CHEMOTHERAPY TOXICITIES

Hee Jeung Oh^{a, b, c*}

^a Chemical Engineering, Pennsylvania State University, University Park, USA

^b Materials Science and Engineering, Pennsylvania State University, University Park, USA

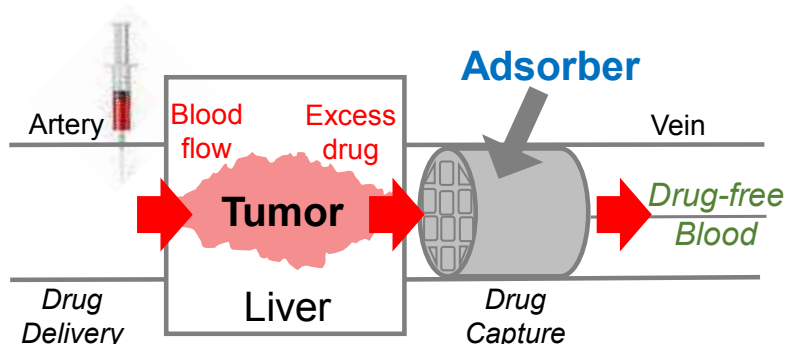
^c 2025 IUPAC Young Observer for the 53rd IUPAC General Assembly and 50th World Chemistry Congress the U.S. National Committee (USNC)

*Corresponding author: hjoh@psu.edu

Abstract

Cancer is the leading cause of death in most developed nations. Despite the effort to develop targeted and personalized chemotherapy drugs, the dosing of drugs is limited by toxic side effects. More than 90% of the injected chemotherapy drug, regardless of injected amount, is not trapped by a target organ, goes to the heart, and circulates throughout the body. In the context of reducing chemotherapy toxicities, we have designed biosponge adsorbers that can selectively bind to target ionic chemotherapy drugs. In this work, we aim to understand the governing transport mechanism of ionic chemotherapy drugs in charged nanostructured block copolymer membranes with different ion-exchange capacities (IECs) and equilibrium water swelling. Sulfonated styrenic pentablock copolymers are used as a model polymer, and doxorubicin (dox) is used as a model chemotherapy drug. We performed a cycle of drug sorption/desorption experiments to quantify the amount of free-dox and bound-dox in the sulfonated polymer membranes. Upon this work, we aim to understand the design principles of charged biosponge block copolymers for different ionic chemotherapy drugs. Designing highly selective biosponge polymer adsorbers can effectively remove untrapped chemotherapy drugs in the body, and thus, can help patients fight cancer.

Keywords: Membrane, charged polymer, drug capture, chemotherapy, doxorubicin, biosponge, 3D printing



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THE POTENTIAL TRILLION-RINGGIT ECONOMY TREASURE OF PALM OIL VITAMIN E INDUSTRY

Hew Nam Fong^{a,*}

^aChM. Dr. Hew Enterprise.

**Corresponding author: hewnf1241@gmail.com*

Abstract

Palm oil contains about 1,000 ppm or 0.1% vitamin E by weight, which composed of mainly α -tocopherol, α -tocotrienol, γ -tocotrienol, and δ -tocotrienol. It is known that these natural vitamin E isoforms possess a huge number of physiological properties and clinical effects, which are related to their excellent antioxidant activities and coenzyme functions. Considering the annual total production of crude palm oil in Malaysia as 20 million tonnes, its total content of vitamin E will be about 20,000 tonnes, isolation of 50% of the vitamin E and separation into pure isoforms may contribute 50 billion ringgits market values from their supplement and pharmaceutical products. In another calculation for comparison, 500 g of vitamin E extracted and separated from every tonne of crude palm oil would raise an extra revenue of RM2,500 to the palm oil industry, unfortunately this lucrative potential has been ignored in the past few decades, probably due to impractical technology on the purification of pure vitamin E isoforms and lack in application research especially on the tocotrienols. This paper will describe that, isolation and purification of individual tocotrienols at pilot scales have been achieved more than three decades ago. In addition, various other phytochemicals such as squalene and phytosterols are also isolable for health and medical uses. Hopefully in the near future, mass production of vitamin E and phytochemicals from palm oil and oil palm leaves would be materialized for various pharmaceutical and therapeutic applications. A fundamental homeostasis theory of vitamin E would also be presented.

Keywords: Palm oil phytochemicals, vitamin E, tocopherol, tocotrienol, fundamental homeostasis theory

SYNTHESIS, ANTITRYPANOSOMAL ACTIVITY, ADME AND DNA BINDING OF BENZOTHAIAZOLE AMIDOXIMES AND ARYLIMIDAMIDES

Silvana Raić-Malić^{a*}, Valentina Rep Kaulić^a, Martina Piškor^a, Sanja Koštrun^b, Astrid Milić^b,
 Marijana Radić Stojković^c, Amanda Fortes Francisco^d,
 Martin C. Taylor^d, John M. Kelly^d

^aUniversity of Zagreb, Faculty of Chemical Engineering and Technology

^bSelvita d.o.o.

^cRuđer Bošković Institute, Division of Organic Chemistry and Biochemistry

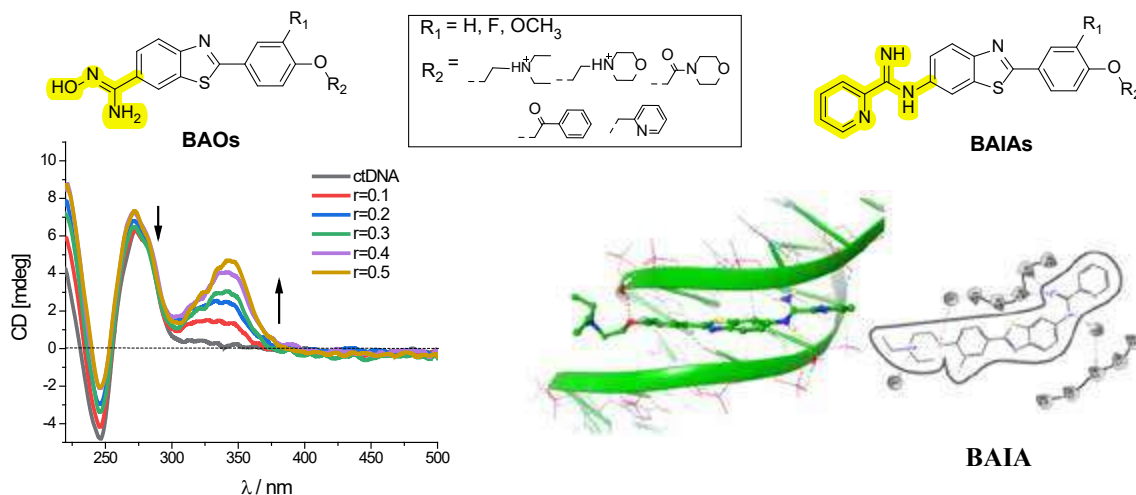
^dDepartment of Infection Biology, London School of Hygiene and Tropical Medicine

*Corresponding author: sraic@fkit.unizg.hr

Abstract

Recently, studies on benzazoles and their amidino derivatives have been conducted to investigate their activity against *Trypanosoma brucei*, the causative agent of African trypanosomiasis.¹⁻⁴ Herein, we have explored structural modifications with the aim to improve the ADME and physicochemical properties of the benzothiazole derivatives and provide a compound suitable for *in vivo* study. Benzothiazole analogues containing 6-amidoxime (**BAOs**) and 6-arylimidamide (**BAIAs**) in place of the amidine moiety, together with aromatic and aliphatic units at the phenoxymethylene were designed and synthesised. Binding strength and mode of binding to DNA/RNA was assessed. Furthermore, physicochemical properties were compared with measured *in vitro* ADME properties, microsomal metabolic stability and membrane permeability. The benzothiazole amidoxime (**BAO**) with diethylaminoethyl and fluorine substituent on a phenoxymethylene linker that exhibited selective antitrypanosomal activity and favourable ADME was submitted to *in vivo* evaluation.

Keywords: benzothiazole, antitrypanosomal activity, ADME, DNA/RNA binding



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CARNOSINE: A PROMISING CHAMPION MOLECULE FOR COMBATING TYPE 2 DIABETES

Charlie A. Lavilla Jr.^{a,*}, Merell P. Billacura^b, Mark D. Turner^c,

^aMindanao State University – Iligan Institute of Technology, Iligan City, Philippines.

^bMindanao State University – Main Campus, Maraw City, Lanao del Norte.

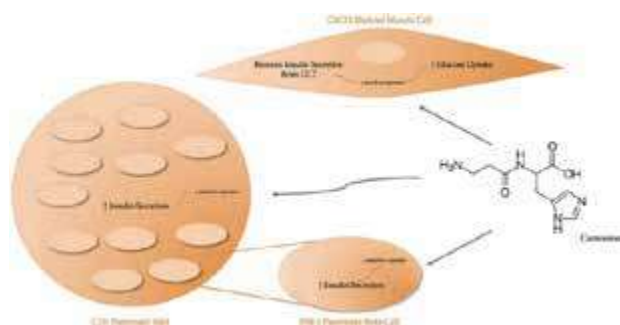
^cNottingham Trent University, UK.

*Corresponding author: charliejr.lavilla@g.msuiit.edu.ph

Abstract

Type 2 diabetes (T2D) is a metabolic disorder characterized by chronically elevated blood glucose levels, insulin resistance, and decreasing insulin secretion from the pancreas, with numerous diabetic complications attributable to the resulting exposure of cells and tissues to chronically elevated concentrations of glucose and fatty acids. This, in part, results from the formation of advanced glycation and advanced lipidation end-products that can modify protein, lipid, or DNA structure, and disrupt normal cellular function. Worryingly, the incidence of diabetes continues to grow at an alarming rate, with the projected figure rising from an estimated 451 million adults worldwide in 2017, to 693 million by 2045. Therapeutic strategies to treat T2D have mainly focused on metabolic aspects of the disease. However, there are a limited number of metabolic targets and the efficacy of pharmacological agents aimed at these targets often becomes less effective over time. This has led to a search for alternative strategies, with one such approach being to try to reduce the oxidative stress that results from chronic exposure to high glucose and fatty acid levels in obesity and T2D. Herein we used mass spectrometry to identify proteins modified by 4-hydroxynonenal (4-HNE) and 3-nitrotyrosine (3-NT) protein adduction events in human serum from patients with obesity, T2D, and gestational diabetes along with similar analyses of human and mouse skeletal muscle cells and mouse pancreatic islets exposed to glucolipotoxic stress, and determined the effect on mitochondrial respiration, and performed GLUT4 translocation assays to quantify the impact on stimulus-secretion coupling in these cells. We also report that carnosine, a histidine-containing dipeptide, prevented 65–90% of 4-hydroxynonenal and 3-nitrotyrosine adduction events and that this in turn preserved mitochondrial function and protected stimulus-secretion coupling in cells exposed to metabolic stress. Carnosine therefore offers significant therapeutic potential against metabolic diseases.

Keywords: type 2 diabetes, obesity, glucolipotoxicity, reactive species scavenging, GLUT4 translocation



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PHOTOCYTOTOXIC EVALUATION AND ISOLATION OF CHEMICALS FROM STROBILANTHES CRISPA (L.) BLUME LEAF EXTRACTS AGAINST SKIN CANCER CELLS

Chee-Shien Chen^a, Chui-Fung Loke^b, Tze-Ven Poh^c, Oi-Ming Lai^d, Siow-Ping Tan^{a*}

^aDepartment of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, 53300 Kuala Lumpur, Malaysia

^bResearch & Development and Commercialization, Tunku Abdul Rahman University Management and Technology, 53300 Kuala Lumpur, Malaysia

^cDepartment of Computer Science and Embedded Systems, Faculty of Computing and Information Technology, Tunku Abdul Rahman University Management and Technology, 53300 Kuala Lumpur, Malaysia

^dFaculty of Biotechnology and Biomolecular Sciences, Universiti Putra Malaysia, 43400 Selangor, Malaysia

*Corresponding author: tansp@tarc.edu.my

Abstract

Strobilanthes crispa (L.) Blume (*S. crispa*) is a widely recognized folklore medicinal plant, known for its diverse range of traditional uses and pharmacological properties. With proven anticancer properties on various cancer cell types, its effect on skin cancer cells remains unclear. This study aims to evaluate the photocytotoxicity of *S. crispa* leaf extracts against the A431 human skin squamous carcinoma cell line using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay, as well as to isolate and identify potential bioactive phytochemicals through various chromatographic and spectroscopic methods. Upon activation with photodynamic therapy (PDT) treatment, cell viability decreased, with the hexane crude extract exhibiting the highest photocytotoxic activity against the A431 cell line (IC₅₀ value of 6.06 ± 0.21 µg/mL), followed by the ethanolic crude extract (IC₅₀ = 8.83 ± 0.55 µg/mL) and the ethyl acetate crude extract (IC₅₀ = 9.37 ± 0.71 µg/mL). However, in the absence of PDT treatment, all three crude extracts demonstrated no significant activity against the A431 cell line, even at concentrations up to 200 µg/mL after 24 hours of dark incubation. This findings suggest that *S. crispa* could serve as a significant source of photosensitizing agents for PDT-based skin cancer treatment. Hence, further isolation and characterization of its bioactive compounds have been carried out. To date, two phytochemicals have been successfully isolated from hexane crude extract, and further studies are needed to evaluate their potential as photosensitizers in skin cancer treatment.

Keywords: *Strobilanthes crispa*, Photocytotoxicity, PDT treatment, A431 cells, MTT assay

TOXICOLOGICAL EVALUATION OF CUCUR ATAP EXTRACT IN RATS: A FIXED-DOSE STUDY UNDER OECD GUIDELINE 420

Teh Bee Ping^{a,*}, Azlina Zulkapli^a, Siti Zubaidah Che Lem^a, Suganthi Jeyabalan^a, Maizatul Hasyima Omar^a, Amirrudin Muhammad^a, Tavinraj Rajendran^a, Nurulfariza Ramli^a, Wan Mohamad Adham Afiq Wan Zainuzzaman^a, Zahra Afni Ahmad^a, Siau Thien Chen^a, Dalnitha Lea Nichol^a, Muhd Zaim Mohamad Akhir^a, Voon Yee Lin^a, Mohd Ridzuan Mohd Abd Razak^a, Norizah Awang^a, Ami Fazlin Syed Mohamed^a

^aNon-Clinical Research Facility, Good Laboratory Practice Section, Institute for Medical Research, 50588 Jalan Pahang, Wilayah Persekutuan Kuala Lumpur, Malaysia.

*Corresponding author: tehbp@moh.gov.my

Abstract

Conducting toxicity assessments in compliance with Good Laboratory Practice (GLP) is essential to ensure the quality, reliability, and credibility of the study findings, which are accepted by regulatory bodies and trusted by the scientific community. *Baeckea frutescens* (commonly known as cucur atap) is a shrub native to Malaysia. Its leaves are traditionally brewed into herbal tea to stimulate menstrual flow, applied during childbirth, and used to treat fevers and boost energy. This study aimed to evaluate the acute toxicity of cucur atap extract following a single oral administration in female Sprague Dawley rats, with observations for 14 days. The experiment adhered to OECD Guideline No. 420, using an initial dose of 300 mg/kg and a highest dose of 2,000 mg/kg body weight. Six female rats were tested, and no mortality, morbidity, or signs of toxicity were observed. Weekly increases in body weight, food intake, and water consumption were noted but not statistically analysed due to the absence of a control group. Gross organ examinations revealed no signs of toxic effects. Consequently, the approximate lethal dose (LD₅₀) was estimated to be above 2,000 mg/kg, classifying the test item as Category 5/Unclassified under the Globally Harmonised System (GHS). Despite the valuable insights provided by this study, its limitations such as the single-dose design and short duration, necessitate further research with repeated dosing.

Keywords: good laboratory practice, OECD, acute toxicity, cucur atap, *Baeckea frutescens*



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DEVELOPMENT OF HYPOXIA-ACTIVATED PRODRUGS OF SECOND-GENERATION ANALOGUES OF BEDAQUILINE FOR TREATMENT OF LATENT TUBERCULOSIS

Christine Kim^a, Jiney Jose^a, Michael Hay^a, Peter Choi^{a*},
^a*Auckland Cancer Society Research Centre, University of Auckland.*
^{*}*Corresponding author: p.choi@auckland.ac.nz*

Abstract

Latent tuberculosis (TB) is one of the main mechanisms of TB virulence. It can survive in the host for decades, and only becomes active when the host becomes immunocompromised. Granulomas are the pathological hallmark of TB that are formed when the adaptive immune system contains *Mycobacterium tuberculosis* (Mtb). Hypoxia is an element of granulomas and causes Mtb to turn latent. Granulomas compromise effective delivery of oxygen and TB drugs, and this emphasises the need to treat latent TB in hypoxic environments.^{1,2} Bedaquiline was approved by the FDA in 2012 for the treatment of multidrug-resistant TB. It demonstrates excellent efficacy against Mtb, but a few adverse effects such as QT prolongation have led to the development of improved second-generation analogues. The best second generation analogues were TBAJ-587 and TBAJ-876 which are currently in human clinical trials.^{3,4,5}

The main objective of our study is to develop and explore a hypoxia-activated prodrug (HAP) strategy to deliver bedaquiline, TBAJ-587 and TBAJ-876 to hypoxic regions in granulomas to increase selectivity and reduce toxicity. Here we present novel protocols for the synthesis of thirty-six HAPs of bedaquiline, TBAJ-587 and TBAJ-876. The compounds were tested for anti-TB activity in both Microplate Alamar Blue Assay (MABA) and Low-Oxygen Recovery Assay (LORA). Initial biological results demonstrate these prodrugs show selectivity towards Mtb under hypoxic conditions highlighting evidence of selective hypoxia-mediated release. The susceptibility data for HAPs demonstrates comparable activity with that of the corresponding parent drugs. Further biological testing of HAPs in intramacrophage mouse infection model is scheduled. These results will provide valuable insights into developing novel HAP strategies for the treatment of TB.

Keywords: Antibiotics, Prodrugs, *Mycobacterium Tuberculosis*, bioactivation, Diarylquinolines

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PRELIMINARY STUDY OF ELEMENTAL ANALYSIS OF ILLICIT TOBACCO PRODUCTS FROM SELECTED COUNTRIES

Ujang Tinggi^{a,b,*}, Mark Myerson^c, Madeleine Farrell^b, Taylor Sillcock^b, Jim Carter^b,
Stephen Finalyson^b, Bruce Morton^b

^aGriffith University, School of Pharmacy and Medical Sciences

^bQueensland Health, Public Health and Scientific Services

^cQueensland Health, West Morton Public and Environmental Health

*Corresponding author: u.tinggi@griffith.edu.au; ujang.tinggi@health.qld.gov.au

Abstract

It is well documented that tobacco smoke has severe health impacts such as increased incidence of cardiovascular diseases, lung cancer and other respiratory diseases ¹. In addition to harmful chemicals such as nitrosamines, hydrocarbons and aldehydes, tobacco products have been reported to contain various levels of toxic heavy metals, including Pb and Cd ^{2,3,4}. The aims of this study were to analyze a wide range of heavy metals (Al, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Sr, Mo, Cd, Hg, Pb) in tobacco products to assess health impacts and to evaluate product origin by comparing the elemental profiles between countries. The samples were obtained from retail outlets in Queensland, Australia. Elemental analysis of initial samples (n=27) was performed using ICP-MS (Agilent 8900) after microwave digestion. Further study will also be conducted on the levels of stable isotope ratios (⁸⁷Sr/⁸⁶Sr, ¹³C/¹²C, ¹⁵N/¹⁴N, ²H/¹H) for identifying and validating the provenance of the products. The preliminary results have shown a wide variation of elemental levels in tobacco products from different countries. High levels were found for Al (118-438 mg/kg), Mn (122-2215 mg/kg), Zn (22-117 mg/kg) and Sr (28-130 mg/kg). Relatively high levels were found for toxic metals of Cd (0.24-19.6 mg/kg) and Pb (0.24-1.57 mg/kg), and low for As (0.03-1.05 mg/kg) and Hg (<0.005-0.067 mg/kg). The results have also shown significant correlations between some elements in these tobacco products. High correlations were found for Al and V (r=0.94), Al and Fe (r=0.93), Cr and Ti (r=0.85), Mn and Zn (r=0.97), Se and Co (r=0.99), Cd and Mn (r=0.96) and Pb and As (r=0.72). Analysis of isotope ratios (Sr, C, N, H) will be evaluated to identify the origin of the tobacco products.

Keywords: heavy metals, tobacco, isotope ratios, ICP-MS

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DEVELOPMENT OF A NOVEL FLUORESCENT PROBE FOR THE SENSITIVE DETECTION OF GLUTATHIONE IN BIOLOGICAL FLUIDS

Ali O. Alqarni^a, Hamdi Mohamed^b, Ashraf M. Mahmoud^a, Al-Montaser Bellah H. Ali^b

^a *Department of Pharmaceutical Chemistry, College of Pharmacy, Najran University, Najran, Saudi Arabia*

^b *Department of Pharmaceutical Analytical Chemistry, Faculty of Pharmacy, Assiut University, Assiut, Egypt*

**Corresponding author: aokalqarni@nu.edu.sa*

Abstract

This study presents the development of a novel fluorescent probe for the sensitive detection of glutathione (GSH), a critical tripeptide thiol that plays essential roles in maintaining cellular redox homeostasis, detoxification processes, and protection against oxidative stress. Given glutathione's significance as a biomarker for various pathological conditions including cancer, neurodegenerative disorders, and cardiovascular diseases, reliable methods for its determination in biological systems are of paramount importance. The fluorescent probe was synthesized through a three-step process beginning with ethyl 5-acetamido-1,2,4-triazole-3-carboxylate. This ester was subjected to reaction with hydrazine to yield the corresponding hydrazide intermediate, which was subsequently condensed with salicylaldehyde to afford the target hydrazone-based probe in high yield. The resulting compound demonstrated excellent photophysical properties, including a remarkable quantum yield of 32.25%, enabling highly sensitive detection capabilities. The probe exhibited selective fluorescence enhancement in the presence of glutathione over other biologically relevant analytes, with a linear response across physiologically relevant concentrations. Validation studies confirmed the probe's applicability for glutathione quantification in complex biological matrices, including human serum and cellular extracts, with excellent recovery rates and precision. This new fluorescent tool offers significant advantages for glutathione monitoring in biological systems, potentially advancing both clinical diagnostics and fundamental research in redox biology.

Keywords: fluorescent probe, glutathione, biological fluids, detoxification processes, neurodegenerative

KRATOM ALKALOIDS: BLOOD-BRAIN AND INTESTINAL BARRIER INTERACTIONS

Nur Aziah Hanapi^{a,*}, Nelson Jeng-Yeou Chear^a, Siti Rafidah Yusof^a,

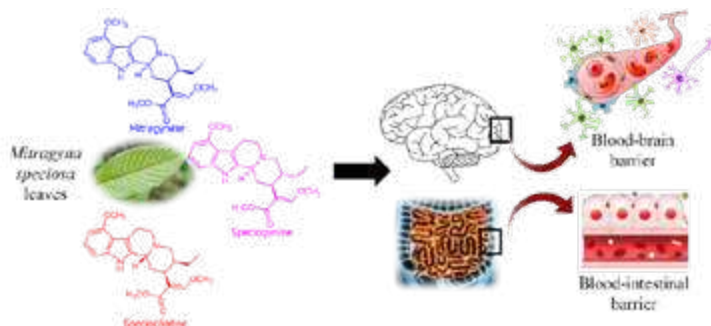
^aCentre for Drug Research, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

*Corresponding author: aziah.hanapi@usm.my

Abstract

Kratom is a tropical evergreen tree native to Southeast Asia of which the leaves have been used for centuries in traditional medicine. Kratom's enduring relevance potentially lies in its alkaloids with reported polypharmacological central actions, particularly mitragynine, 7-hydroxymitragynine, speciogynine, and speciociliatine. Despite a wealth of evidence on the pharmacological actions of these compounds, a significant knowledge gap remains regarding their interactions with cellular barriers including the blood-brain barrier (BBB) and the blood-intestinal barrier, i.e. the key determinants of central nervous system (CNS) drug efficacy and oral absorption. Seeking to illuminate the brain and intestinal permeability characteristics of these alkaloids, this study utilized *in vitro* models of the BBB, and the intestinal barrier established using primary porcine brain endothelial cells and the Caco-2 cells, respectively. Our previous work, focusing on mitragynine and 7-hydroxymitragynine, revealed distinct BBB permeability profiles between the two alkaloids. While mitragynine showed higher permeability than 7-hydroxymitragynine, the latter showed higher unbound fraction in the brain which potentially explains its higher antinociceptive potency than mitragynine¹. Building upon this data, the current study examined the BBB permeability of speciogynine and speciociliatine, where both were found to show similar BBB permeability to mitragynine². The apparent permeability (P_{app}) values of these alkaloids suggest a shared potential for CNS penetration, comparable to CNS-drug like molecules. However, different observations were made at the intestinal level. Mitragynine and speciogynine displayed moderate intestinal permeability. On the other hand, speciociliatine exhibited significantly lower permeability, hinting at limited intestinal uptake². This disparity highlights the complex interplay between the chemical structures of these alkaloids and biological barriers. While speciociliatine's limited intestinal permeability may restrict its oral bioavailability, its robust BBB permeability suggests a promising avenue for CNS drug development. Similarly, the comparable BBB permeability and moderate intestinal permeability of speciogynine and mitragynine reinforce their potential as CNS therapeutic candidates.

Keywords: Blood-brain barrier, intestinal barrier, mitragynine, speciogynine, speciociliatine



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DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION OF NOVEL TRIFLUOROMETHYLATED IMIDAZONAPHTHYRIDINE DERIVATIVES AS POTENTIAL ANTIMICROBIAL AGENTS

Wong Siew Fang^a, Koh Zhan Ning^a, Goh Joo Kheng^{a,*}

^a*School of Science, Monash University Malaysia, Jalan Lagoon Selatan, 47500 Bandar Sunway, Selangor Darul Ehsan, Malaysia*

^{*}*Corresponding author: goh.joo.kheng@monash.edu*

Abstract

The rise of multidrug-resistant bacteria has created an urgent demand for novel antimicrobial agents to combat life-threatening infections. Antibiotic resistance, largely driven by misuse, overuse, and unrestricted access, poses a severe global threat. The World Health Organization (WHO) has identified 12 bacterial families with limited treatment options, warning of a potential post-antibiotic era in which even minor infections could become fatal. Addressing this crisis requires the development of antimicrobial agents with distinct chemical frameworks and mechanisms of action. Fused imidazonaphthyridine compounds have recently gained attention in medicinal and synthetic organic chemistry due to their diverse biological activities, including anti-inflammatory, antiviral, and anti-hepatitis properties.¹ Building on their pharmacological potential, the design, synthesis, and biological evaluation of trifluoromethylated (CF₃)-imidazonaphthyridine derivatives as potential antimicrobial agents are undertaken in this study. The synthesized compounds will be structurally characterized and screened *in vitro* against clinically significant Gram-positive and Gram-negative bacteria. It is hypothesized that the synthesized derivatives will exhibit antimicrobial activity within the tested concentration range (2–256 µg/mL). By expanding the repertoire of antimicrobial candidates, this research may contribute to the development of alternative treatment options in response to escalating antibiotic resistance. The findings could provide valuable insights into pharmaceutical and medicinal chemistry, paving the way for innovative therapeutic strategies against bacterial infections.

Keywords: imidazonaphthyridine, heterocyclic scaffold, synthesis mechanism, biological activity

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PHYSALIA PHYSALIS JELLYFISH COMPONENTS: PEPSIN-SOLUBILIZED COLLAGEN CHARACTERIZATION AND POLYPHENOLS COMPOSITION

Ferreira Inês ^{a,b,*}, Pires Carla ^{b,c}, Silva Andreia ^d, Bandarra Narcisa ^{b,c}, P. Rauter Amélia ^a and Bronze Rosário ^d

^a Centro de Química Estrutural, Institute of Molecular Sciences, CiênciasULisboa,

^b Division of Aquaculture, Upgrading and Bioprospecting, IPMA

^c Interdisciplinary Centre of Marine and Environmental Research (CIIMAR), University of Porto

^d Faculdade de Farmácia, Universidade de Lisboa

*Corresponding author: fc53396@alunos.fc.ul.pt

Abstract

Jellyfish bloom is a huge concern to human health due to more than 150 million stings worldwide, which can cause pain, nausea, vomiting or respiratory distress and death (1). *Physalia physalis* (Fig 1) is one of the most venomous jellyfish in the world. In the last five years, many first reports on *Physalia physalis* occurrences in several countries have been published (2,3). This harmful jellyfish is an unexplored marine source with a negative socioeconomic impact. We have been studying *P. Physalis*, focusing its valorization on oceanic biodiversity and conservation, human health and global economic problems. Based on the known methodology for jellyfish species (4), we succeeded in carrying out pepsin-solubilized collagen extraction from the pneumatophore and have also investigated *P. physalis* polyphenols composition. Collagen has been characterized by electrophoresis giving us its molecular weight and collagen composition. Major amino acids in collagen extracts of *P. physalis* pneumatophore were glycine, proline and aspartic acid. Collagen of pneumatophore revealed a similar pattern to collagen type I, which is extracted nowadays from mammalian sources and used in human consumption and health. Tentacles polyphenols have been identified by HPLC and HPLC-MS. A large spectrum of polyphenols was found, including gallic acid, gallic acid gallate, *m*-coumaric acid succinic acid. These results are, indeed, a promising start for the valorization of this specie contributing to the Blue Economy.

Keywords: Blue economy; Jellyfish; *Physalia physalis*; Collagen; Polyphenols



Figure 1.
Physalia physalis



Figure 2.
Physalia physalis bloom

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FROM SYNTHESIS TO HUMAN HEALTH: EXPLORING QUINAZOLINE DERIVATIVES FOR MULTITARGET NEUROLOGICAL AND INFECTIOUS DISEASE THERAPY

Nishtha^{a*}, Manish Kumar^a, Neelam Sharma^b, Vijay Sharma^a

^a*Dr. K. N. Modi Institute of Pharmaceutical Education and Research, Modinagar, Ghaziabad, Uttar Pradesh-201204, India.*

^b*Department of Pharmaceutical Chemistry, Shri Ram College of Pharmacy, Indri Road, Ramba, Karnal, Haryana-132116, India.*

^{*}*Corresponding author: nishtha.sch@jamiahamdard.ac.in*

Abstract

Quinazoline is a well-known pharmacophore with diverse biological activities. Developing multifunctional derivatives with anticonvulsant and antimicrobial potential is of growing interest due to the increasing need for safer and more effective therapies. This study aimed to synthesize novel 3-substituted quinazoline-2,4-dione derivatives and evaluate their anticonvulsant, antibacterial, and antifungal activities, supported by molecular docking studies. A series of 3-substituted quinazoline-2,4-dione compounds were synthesized using standard chemical methods.

- **Anticonvulsant activity** was tested using the maximal electroshock seizure (MES) model in mice at a dose of 30 mg/kg.
- **Antimicrobial activity** was evaluated against Gram-positive (*B. subtilis*, *S. aureus*), Gram-negative (*E. coli*, *P. aeruginosa*), and fungal strains (*C. albicans*, *A. niger*) using the agar well diffusion method (100 µg/mL).
- **Molecular docking** was performed with target proteins: 2Z5X (GABA-A receptor), 6BPP (bacterial topoisomerase IV), and 7VPR (fungal lanosterol demethylase).
- **Compound 4h** showed significant anticonvulsant activity, comparable to phenytoin sodium.
- **Compound 4f** demonstrated broad-spectrum antibacterial activity against all tested strains.
- **Compound 4b** showed strong antifungal activity, outperforming griseofulvin.
- Docking studies confirmed strong binding affinities of these active compounds with key residues at respective target sites.

The synthesized 3-substituted quinazoline-2,4-dione derivatives, particularly compounds 4h, 4f, and 4b, exhibited promising anticonvulsant and antimicrobial activities. These results suggest their potential as lead compounds for further development of multi-target therapeutic agents.

Keywords: Quinazoline, anticonvulsant, antimicrobial, antifungal, molecular docking

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DESIGN, SYNTHESIS AND MECHANISTIC STUDIES OF BENZIMIDAZOLES AS A NOVEL CLASS OF THERAPUETICS AGAINST DRUG-RESISTANT ORAL CANCER CELLS

Muhammad Azri Faiz Abd Zaki,^a Wai Leng Lee,^a Hock Siew Tan,^a Keng Yoon Yeong^{a*}

^a*School of Science, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, 47500 Selangor, Malaysia.*

**Corresponding author: yeong.kengyoon@monash.edu*

Abstract

Utilising compounds which target novel cancer-related protein such as sirtuins represents a promising strategy in combating drug-resistant oral cancer. Although benzimidazoles have consistently drawn attention as potential anticancer agent, current treatments for oral cancer do not incorporate the benzimidazole scaffold. This highlights bioactive benzimidazoles as a compelling scaffold for exploration in the development of oral cancer therapeutics, especially for those targeting resistant cancer. Following the anticancer property exhibited by our previously reported benzimidazole-based sirtuin inhibitor BZD9Q1, structural modifications were carried out to improve potency and metabolic stability. Among the newly synthesized molecules, compound **7k** exhibited the best anticancer activity against cisplatin-sensitive H103 oral squamous carcinoma cells (OSCC) ($IC_{50} = 2.35 \mu M$). Additionally, it also demonstrates significant anticancer activity against cisplatin-resistant (H103cisD2, H314) cell lines. Compound **7k** exerted its activity by arresting H103cisD2 cells at the G2/M checkpoint and inducing late apoptosis to reduce the cell viability. Meanwhile, differential gene analysis revealed that the cell death conferred by compound **7k** may be induced through endoplasmic reticulum (ER) stress.

Keywords: Benzimidazole; anticancer; oral cancer; resistant; ER stress

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DIETARY SUPPLEMENTATION WITH *EUCHEUMA DENTICULATUM* ALTERS PLASMA METABOLITES IN HIGH-FAT DIET-FED RATS: AN NMR-BASED METABOLOMIC STUDY

Vimala Balasubramaniam*, Mohd Naeem Bin Mohd Naw, Siti Khadijah Binti Abdul Khalid

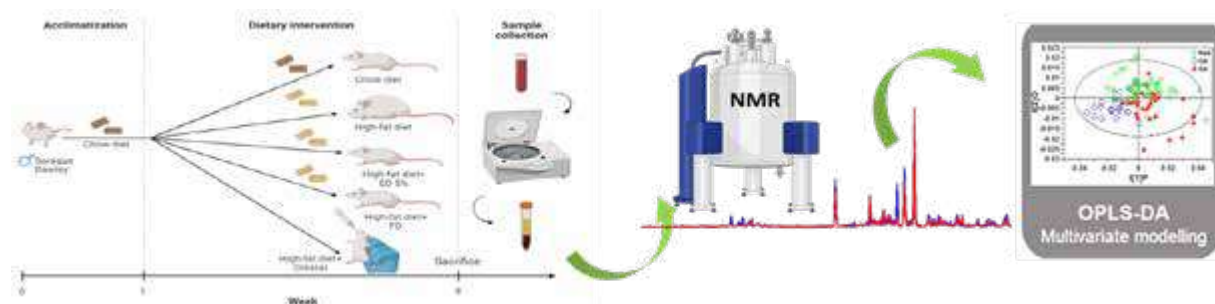
Nutrition, Metabolism & Cardiovascular Research Centre, Institute for Medical Research, National Institute of Health, Ministry of Health, Block C7, Level 3, No.1, Jalan Setia Murni U13/52, Seksyen U13, Setia Alam, 40170 Shah Alam, Selangor, Malaysia

*Corresponding author: vimala.rmt@moh.gov.my

Abstract

Eucheuma denticulatum (ED), a red seaweed commonly found along the Sabah coastline, has demonstrated bioactive properties with potential anti-obesity effects^{1–3}. This study aimed to evaluate the metabolomic effects of ED supplementation in a high-fat diet (HFD)-induced obesity model using ¹H NMR-based metabolomics. Thirty male Sprague Dawley rats were divided into five groups (n = 6): normal diet (ND), HFD, HFD with 5% ED (5ED), a formulated ED beverage (FD), and orlistat (ORL). After 8 weeks of intervention, plasma samples were analyzed by ¹H NMR spectroscopy, and 43 metabolites were identified. The fold change and t-test analyses revealed significantly elevated levels of 3-aminoisobutyrate, 3-hydroxybutyrate, betaine, fucose, and glucose in the HFD group compared to ND (p < 0.05). Supplementation with 5ED significantly altered key metabolites such as arginine, pyruvate, and TMAO (p < 0.05, fold change > 2), suggesting a reversal of HFD-induced metabolic dysregulation. Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) showed a clear separation between HFD, 5ED, and ORL groups. VIP score analysis (VIP > 1.5) identified citrate, glycylproline, malate, lactate, ornithine, and trans-4-hydroxy-L-proline as major contributors to group discrimination. The FD group showed partial metabolic improvement. These findings highlight the potential of *E. denticulatum*, as a functional food to modulate diet-induced metabolic dysfunction.

Keywords: anti-obesity, *Eucheuma denticulatum*, metabolomics, NMR spectroscopy



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TWO NEWS LIMONIDS FROM *CARAPA PROCERA* SEEDS AND THEIR ANTIMICROBIAL ACTIVITY

Moussa Ndao^{a,d}, Samba Fama Ndoye^b, Ismaila Ciss^a, Seynabou Sokhna^a, Abda Ba^a, Lalla Aicha Ba^c, Insa Seck^b Mehdi Beniddir^d and Matar Seck^a

^a Laboratoire de Chimie Organique et Thérapeutique, Faculté de Médecine, de Pharmacie et d'Odontologie de l'Université Cheikh Anta Diop de Dakar, BP 5005 Dakar-Fann, Sénégal;

^b Laboratoire de Chimie de Coordination Organique (LCCO), Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop de Dakar, Dakar, Sénégal.

^c Université Amadou Mahtar MBOW, BP 45927 Dakar Nafa VDN, Sénégal. Dakar-Fann, Sénégal

^d Laboratoire BioCIS/CNRS, Université Paris Saclay, Paris, France

Abstract

The search for new active ingredients has often relied on plant biodiversity, which is an inexhaustible reserve of bioactive substances with pharmaceutical potential. ⁽¹⁻³⁾ *Carapa procera* is a species of the Meliaceae family with high therapeutic potential, comprising around 50 genera and over 1400 species, ⁽⁴⁾ is found mainly in Africa and Latin America. ⁽⁵⁾ It is mainly found in Casamance and in the forest galleries of eastern Senegal and is widely used in traditional African medicine ⁽⁵⁾. It is one of *Carapa*'s least-literatured species (12 compounds in DNP). The objective of this study is to evaluate the antimicrobial activity of the new isolated compounds. Investigation of ethyl acetate extract of delipidated *C. procera* seeds resulted in isolation of thirteen limonoids. A new azadirone, 6 β ,17 α -dihydroxyazadiradione (**1**) and a new gedunin, 5-hydroxy-7-deacetoxy-7-oxogedunin (**2**) were isolated from *C. procera* seeds, together with eleven known compounds, krishnagranatin C (**3**), 6-deoxydetigloylswietenin (**4**), mexicanolide (**5**), 7-deacetylgedunin (**6**), Khayasin (**7**), xylomexicanolide A (**8**), 14,15-didehydroruageanin A (**9**), andiolide A (**10**), swietmanin H (**11**), 17 β -dihydroxyazadiradione (**12**) and 6 α -hydroxyazadiradione (**13**). Their structures were assigned on the basis of spectroscopic data and their absolute configurations were established by NOESY and X-ray diffraction analysis confirmed by ECD. Antimicrobial activity of four compounds (**1-4**) was evaluated against *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Candida albicans* and *Mycobacterium marinum*. 6-deoxydetigloylswietenin (**4**) was the most active among them and the only one active against *Mycobacterium marinum* with MIC 0.21 mM. These results demonstrate that *C. procera* parts are rich in bioactive compounds, validating its use in traditional medicine.

Keywords: *Carapa procera*, antimicrobial activity, phytochemical screening

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TINY DROPLETS, BIG IMPACT: NANOEMULSION OF LUTEIN AND ZEAXANTHIN FOR VISION PROTECTION

Nicholas Peh Hian Tunga*, Wei Meng Limb, Yun Khoon Liewc, Chaw Jiang Limd, Yoon Yee Thene, Kok Whye Cheongf, Lai Chun Wonge*

*a*Centre for Postgraduate Studies by Research, IMU University, 57000 Kuala Lumpur, Malaysia

*b*Department of Life Sciences, School of Pharmacy, Monash University, 47500 Subang Jaya, Malaysia

*c*Department of Life Sciences, School of Pharmacy, IMU University, 57000 Kuala Lumpur, Malaysia

*d*Department of Chemical Science, Faculty of Science, University Tunku Abdul Rahman, 31900 Kampar, Malaysia

*e*Department of Pharmaceutical Chemistry, School of Pharmacy, IMU University, 57000 Kuala Lumpur, Malaysia

*f*Department of Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, UCSI University, 56000 Kuala Lumpur, Malaysia

*Corresponding authors: pehnic@yahoo.com; wlaichun@yahoo.com

Abstract

Vision impairment affects approximately 2.2 billion people globally, with cataracts, glaucoma, and age-related macular degeneration being the leading causes 1. These conditions are often linked to oxidative stress and age-related degeneration of ocular tissues 2. Lutein and zeaxanthin are dietary carotenoids highly concentrated in the macula, known for their antioxidant and anti-inflammatory properties 3. They play a protective role in ocular health but suffer from poor water solubility and limited bioavailability. This study aims to develop and characterize nanoemulsion formulation to enhance the ocular delivery and bioavailability of lutein and zeaxanthin for the prevention or management of age-related eye diseases. Lutein and zeaxanthin were incorporated into an oil-in-water nanoemulsion system using a high-energy emulsification technique. Formulation parameters were optimized using response surface methodology. The nanoemulsion was evaluated for droplet size, polydispersity index, zeta potential, and physical stability. The optimized nanoemulsion exhibited a mean droplet size of less than 200 nm, and narrow PDI (<0.4). The formulation remained physically stable over three weeks at room temperature and five weeks in the fridge. In conclusion, the developed nanoemulsion holds promise as a non-invasive therapeutic strategy for promoting eye health and reducing the risk or progression of age-related ocular disorders.

Keywords: lutein, zeaxanthin, nanoemulsion, ocular delivery, visual impairment

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NEUROPROTECTIVE PROPERTIES OF PLANT-DERIVED BIOACTIVE COMPOUNDS: A BIBLIOMETRIC ANALYSIS

Nor Aimi Abdul Wahab^a, Nor Aziyah Bakhari^{b*}, Ainorkhilah Mahmood^c, Nur Iwani Nor Izaham^d, Marina Mokhtar^e, Suhaiza Hasan^f

^{a,b,c,e,f}Department of Applied Sciences, Universiti Teknologi MARA Cawangan Pulau Pinang, Permatang Pauh Campus, 13500 Permatang Pauh, Malaysia

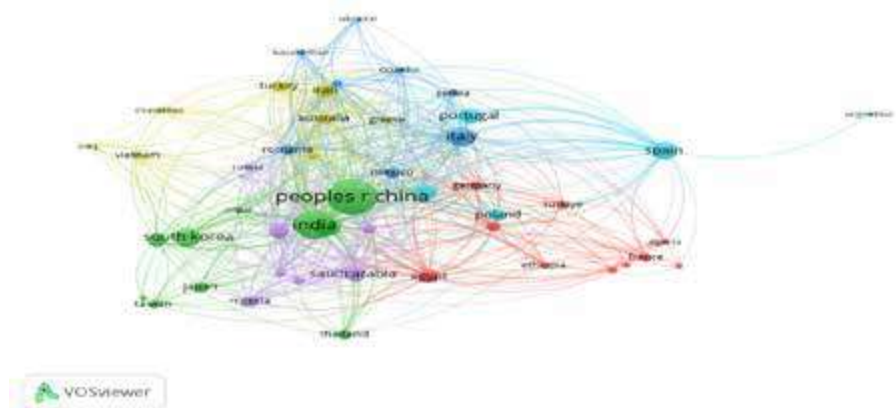
^dFaculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Malaysia

*Corresponding Author: noraziyah140@uitm.edu.my

Abstract

The increased number of people with neurodegenerative diseases (NDs) and the related dementia has in turn prompted an enormous increment in research interest and efforts on the discovery of new therapeutic agents for prevention of these diseases. Numerous medicinal plants have been employed in traditional medical practices to treat cognitive disorders, including memory-related disorders and neurodegenerative diseases like Alzheimer's, Parkinson's and dementia. This paper reports on a bibliometric mapping analysis of publications on the studies of neuroprotective bioactive compounds. Relevant studies associated with the theme were collected from Web of Science database sorted out using predetermined criteria. The study's findings unveil a trend that exhibited an upward total publication trajectory. The number of publications has grown steadily since 2015, with a sharp rise observed particularly over the last five years. The significant growth in publications reflects the increasing scientific attention towards plant-based neuroprotection. A total of 106 countries around the globe have contributed at least one publication on the topic. China exhibited the most substantial contribution, constituting 26.5% from the total of 1144 publications, followed by India at 17.6% and Italy at 8.0%. Network visualization reveals a highly interconnected research landscape, where China, the USA, and European nations act as central players, while countries from Asia, Africa, and Latin America form secondary but growing collaborative networks. The presence of regional clusters suggests research may be influenced by linguistic, cultural, or funding factors.

Keywords: Bioactive Compounds, Bibliometric Analysis, Medicinal Plants, Neuroprotective, Science Mapping



Country Co-Authorship Network

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NATURAL PRODUCTS FROM THE EDIBLE SEAWEED *HALYMENIA HAWAIIANA*

Achara Raksat ^a, Md Samiul Huq Atanu ^a, Karla J. McDermid ^b, Marisa Wall ^c, Boon Loong Chang ^d, Supakit Wongwiwatthanankit ^e, Leng Chee Chang ^{a*}

^aDepartment of Pharmaceutical Sciences, The Daniel K. Inouye College of Pharmacy, University of Hawai‘i at Hilo, Hilo, Hawaii, 96720, United States;

^bDepartment of Marine Science, University of Hawai‘i at Hilo, 200 W. Kawili St., Hilo, Hawai‘i 96720, United States;

^cDaniel K. Inouye U.S. Pacific Basin Agricultural Research Center, Hilo, Hawai‘i, 96720, United States;

^dDepartment of Traditional Chinese Medicine, School of Pharmacy, Management and Science University, Shah Alam, Selangor, Malaysia;

^eDepartment of Pharmacy Practice, The Daniel K. Inouye College of Pharmacy, University of Hawai‘i at Hilo, Hilo, HI, 96720, United States

Abstract

This study examined the chemical components and potential medicinal properties of *Halymenia hawaiiiana*, a marine macroalga that is significant in culinary contexts and has been successfully cultivated in Hawai‘i.¹⁻³ Dried and ground *H. hawaiiiana* was extracted in a sequence using ethyl acetate, methanol, and *n*-butanol. Chromatographic procedures led to the isolation and spectroscopic characterization of thirteen compounds, including two nucleosides, a cytosine analog, five saturated long-chain fatty acids, cholesterol, and two cholesterol derivatives. Among the isolates, compounds **10** and **11**, both featuring peroxide side chains, demonstrated promising antimicrobial activity against *Staphylococcus aureus*, with a minimum inhibitory concentration (MIC) of 8 µg/mL. They also showed MIC values of 32 and 64 µg/mL against methicillin-susceptible *S. aureus*. Furthermore, compounds **9**, **10**, and **11** exhibited significant anti-inflammatory effects by inhibiting lipopolysaccharide (LPS)-induced nitric oxide (NO) production in a cell culture model, with IC₅₀ values ranging from 50.2 to 60.8 µM. These compounds effectively inhibited the generation of reactive oxygen species (ROS) and reactive nitrogen species (RNS) in RAW 264.7 mouse macrophage cells, with IC₅₀ values between 55–73.7 µM, all without exhibiting cytotoxicity. Additionally, compounds **9–11** displayed mild cytotoxicity against the non-small cell lung cancer cell line A549, with compound **10** showing the strongest response (IC₅₀ = 86.1 µM). This research highlights the diverse chemical constituents of *H. hawaiiiana*. Compounds **10** and **11**, particularly due to their peroxide side chains, emerge as promising lead compounds for the development of novel anti-inflammatory and antimicrobial agents.

Keywords: *Halymenia hawaiiiana*, edible seaweed, antibacterial activity, cytotoxicity, non-small cell lung cancer cell line A549

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IMPROVING THE PUBLIC PERCEPTION OF SCIENCE/CHEMISTRY THROUGH SIMPLE EXPERIMENTS CONNECTED WITH DAILY LIFE

Samita Maitra^a and Uday Maitra^{b*}

^a*B.M.S. College of Engineering, Bangalore 560019, India.*

^b*Indian Institute of Science, Bangalore 560012, India*

**maitra@iisc.ac.in*

Abstract

Among high school students, interest in studying natural sciences in general, and in chemistry in particular has been facing a challenge during the past two decades. This issue seems to be a global one. While the reasons are manifold, we believe that the importance of applied science cannot be realized unless a sizable proportion of students pursue higher studies in natural science. To increase awareness in science and chemistry, I have been actively interacting with school children, college students and the public during the past two decades. This is accomplished through lectures, videos and hands-on experiments that connect directly or indirectly to real life. The level of the experiments, and the language used for the explanation are always tailored to the target audience, which works out very well. Currently we both are working together as the number of experiments that are covered during these awareness programs has increased on popular demand. Demonstrating experiments in real time in front of numerous curious students is exciting and each time their enthusiasm is contending. Our recent 5-day workshop for 9th grade school children who were given hands-on training on the use of readily available ingredients to understand fundamental principles of chemistry made us motivated. While we do not have any quantitative data, we invariably get very positive feedback from the students, at times several years later!

In this lecture, we will share our experiences and highlight the importance of choosing relevant experiments and appropriate communication to improve the understanding of science among non-scientific groups.

Keywords: science communication; experimental demonstration;



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APPLYING *PREQUESTIONING* AS A LEARNING STRATEGY

Fun Man Fung^{*a}, Steven C. Pan^b

^aUniversity College Dublin, Ireland

^bNational University of Singapore, Singapore

*Corresponding author: funman.fung@ucd.ie

Abstract

Prequestioning is a learning strategy where students take practice tests on upcoming material and then review the correct answers. While effective in lab studies, it has rarely been tested in real classrooms. In this study, we applied *prequestioning* as an interactive, hands-on activity in a small undergraduate environmental chemistry course. Over 10 lecture sessions, the instructor gave four prequestions on concepts for the next lecture, allowing students to guess answers before revealing the correct ones. Assessments in the following session showed a *prequestioning* effect, with stronger performance on prequestioned concepts compared to non-prequestioned ones in most cases. This benefit highlights *prequestioning*'s potential as a practical and cost-effective method for enhancing learning in undergraduate chemistry and similar courses.

Keywords:

Learning Strategy, Prequestioning, Pretesting, Environmental Chemistry, Retrieval Practice

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EXPLORING THE POTENTIAL OF VIRTUAL REALITY TO HELP STUDENTS LEARN CHEMICAL CONCEPTS

Mauro Mocerino^{a*}, Henry Matovu^b, Dewi Ayu Kencana Ungu^c, Mihye Won^d, David Treagust^e, Ricardo Bruno Hernandez-Alvarado^e, Roy Tasker^f, Chin-Chung Tsai^g

^a Science and Engineering, Curtin University, Australia

^b Science, University of Sydney, Australia

^c Education, Nanyang Technological University, Singapore

^d Education, Monash University, Australia

^e Education, Curtin University, Australia

^f Science, Western Sydney University, Australia

^g Education, National Taiwan Normal University, Taiwan

*Corresponding author: m.mocerino@curtin.edu.au

Abstract

Immersive virtual reality (iVR) offers a powerful educational tool, enabling students and researchers to explore virtual environments that are either inaccessible or difficult to access in the real world. In chemistry education, iVR provides an opportunity to visualize and interact with molecular structures at a level of detail that would be impossible in a traditional classroom. Beyond chemistry, iVR has been applied across a range of disciplines such as astronomy, geology, biology, and medicine. However, the full educational potential of immersive VR remains underexplored.¹ We have developed three immersive VR activities where students actively assemble and explore molecular structures to understand molecular shape, polarity, and intermolecular forces. In these iVR activities, students collaborate and navigate the shared virtual environment to address big questions such as „Why do snowflakes have hexagonal symmetry?“ and „Why does D-phenylalanine taste sweet?“ and „Why are enzymes such good catalysts?“ In this presentation, we will describe the VR learning activities we have developed and share some evaluations of their effectiveness.

Keywords: Immersive virtual reality, Intermolecular forces, H-bonding, Collaborative learning,



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STRUCTURING STUDENT LEARNING EXPERIENCES AND DEVELOPING SKILLS: ALIGNING OUTCOMES, ACTIVITIES, AND ASSESSMENT

Renée Cole*

University of Iowa

*Corresponding author: renee-cole@uiowa.edu

Abstract

There is a clear need to help students become more proficient in skills and science practices that will strengthen the workplace and ultimately help solve worldwide challenges in energy, food, technology, and the environment. While the development of these skills is often a general goal for courses and programs, the cultivation of these skills is seldom explicitly discussed or assessed in the classroom. By ensuring that learning outcomes, assessments, and instructional actions are aligned, instructors provide students with coherent curricular opportunities to develop their knowledge and skills and increase the likelihood that instructional actions are appropriate to achieving the desired learning outcomes. Constructive alignment that supports achievement of skills and science practices requires appropriate tasks designed to engage students and approaches to assessment that provide information to both students and instructors on the skill/practice in addition to the “correctness” of the result. The types of assessment used by an instructor also telegraph to students what is valued in a course. However, in many instances, the lack of alignment between instructional methods and assessment detracts from the added value of engaged student learning environments. Our work has included both the analysis of typical practice, outcomes of professional development designed to support evidence-based instructional practices, and the creation of rubrics designed to assess and provide feedback on skills and science practices.¹⁻³ We have used Marzano’s taxonomy to characterize instructional tasks from a variety of contexts and have extended this work to analyze classroom discourse to investigate how task design can influence student engagement.^{4,5} This work provides insights into how instructors can design and align course components to develop more effective learning environments.

Keywords: Curriculum design, Assessment, Professional Skills, Science Practices



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PROBLEM SOLVING AT THE INTERFACE OF CHEMISTRY AND MATHS – COGNITIVE AND EPISTEMIC CHALLENGES

Sofie Ye^a, Maja Elmgren^a, Magnus Jacobsson^b, Felix M. Ho^{a,*}

^aDepartment of Chemistry – Ångström Laboratory, Uppsala University, Sweden.

^bDepartment of Mathematics, Uppsala University, Sweden.

*Corresponding author: felix.ho@kemi.uu.se

Abstract

Problem solving at the interface of mathematics and other scientific disciplines, including chemistry, presents significant challenges for students across a range of fields.¹ Beyond algorithmic mathematical manipulations, meaningful application and integration of chemical and mathematical knowledge at a conceptual level is essential for constructing models and theories that explain and predict chemical behaviour.²⁻⁴ At a deeper level, the relationship between mathematics and other disciplines in science and engineering, as well as the application of mathematics in these fields, is a topic of research that has attracted increasing attention.⁵

Our recent research³⁻⁴ investigating university chemistry students solving physical chemistry tasks that require varying degrees of integration between chemical and mathematical knowledge will be discussed in this presentation. Building on the mathematical modelling cycle⁶ and the resources framework,⁷ we developed the *extended mathematical modelling cycle*³ (below). It offers a more fine-grained account of the subprocesses that students engage in during the modelling, as well as the cognitive resources, both mathematical and non-mathematical, that they activate. While extra-mathematical input often refers primarily to non-mathematical *disciplinary knowledge* (such as chemical knowledge), our findings suggest that it also includes resources grounded in *situational knowledge*—knowledge about what is typical or appropriate in a given problem context.

In addition, our on-going work targeted at exploring the role of students' *epistemic framing* during mathematisation in the context of unfamiliar chemical phenomena will be presented, revealing students' struggles in making decisions where their expectations and understanding across disciplinary boundaries come into conflict. Questions concerning associated demands on the pedagogical content knowledge of instructors in their teaching practice will also be raised for consideration and discussion.

Keywords: Problem solving, physical chemistry, mathematical modelling, disciplinary interface



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RESEARCH ETHICS IN THE CHEMICAL SCIENCES

Eucharia Oluchi Nwaichi¹, Andala Dickson², Peter Ikechukwu Nwaichi³, & Augustine Agi³

¹ *Department of Biochemistry, University of Port Harcourt, Rivers State, Nigeria*

¹ *Academic Planning, Research & Control Unit, University of Port Harcourt, Rivers State, Nigeria*

² *National Research Fund Kenya*

² *Department of Chemistry, Multimedia University, Kenya.*

³ *Universiti Malaysia Pahang Al-Sultan Abdullah, Lebuhraya Persiaran Tun Khalil Yaakob 26300 Kuantan, Pahang, Malaysia*

**Corresponding author: nodullm@yahoo.com*

Abstract

Research ethics play a crucial role in advancing the chemical sciences while addressing global challenges in health, the environment, and sustainable development. Ethical issues, such as data fabrication, environmental neglect, intellectual property disputes, and misuse of research, undermine the integrity of chemical research and societal trust. This study aims to explore key ethical principles in chemical sciences, identify common ethical dilemmas, and propose strategies to promote ethical practices aligned with sustainability. Through a mixed-method approach, including literature review, case study analysis, and interviews with chemists and policymakers, the study reveals gaps in ethical training, particularly in low- and middle-income countries, and highlights best practices from successful ethical cases. Strengthening ethical frameworks and fostering collaboration between scientists and policymakers are critical to ensuring that chemical research aligns with global sustainability goals. Keywords: Research ethics, Chemical sciences, Sustainability, IUPAC, Ethical frameworks.

Keywords: Research ethics, Chemical sciences, Sustainability, IUPAC, Ethical frameworks

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PRE-SERVICE CHEMISTRY TEACHERS' ACTION COMPETENCE AND SELF-EFFICACY IN TEACHING SUSTAINABILITY

Hazel Joyce M. Ramirez^{a,*}

^a*College of Education, University of the Philippines Diliman*

^{*}*Corresponding author: hmramirez@up.edu.ph*

Abstract

Teacher education institution has a pivotal role in promoting sustainable development by improving teachers' understanding of sustainability concepts and preparing them to serve as effective facilitators of sustainability-oriented learning. Baseline research on pre-service chemistry teachers' perspectives and competencies in sustainability is essential, particularly given the growing global body of research contrasted with the limited literature in developing countries like the Philippines. Drawing from this premise, this research aimed to investigate the pre-service chemistry teachers' action competence and self-efficacy in teaching sustainability as well as to determine their experiences on sustainability. This research utilized a convergent mixed-methods design which involved survey administration and interview sessions. The research participants were 34 pre-service teachers. Findings revealed that participants had relatively high action competence and perceived efficacy in teaching sustainability. Additionally, analysis showed that personal experiences with nature, academic and extra-curricular activities, and media consumption influenced their disposition towards sustainability. Research participants also suggested ways that could help develop their efficacy in teaching sustainability such as integration of sustainability in the curriculum, conduct of workshops and seminars on sustainability, and partnership with communities and organizations. The corroboration of qualitative and quantitative data revealed cross-cutting themes on the experiences of pre-service teachers from different levels of action competence. This research provides valuable insights for improving teacher education programs to better equip pre-service chemistry teachers as proactive agents of change, empowering them to effectively advance sustainability education.

Keywords: pre-service science teachers, chemistry, action competence, efficacy, Education for Sustainable Development

BRIDGING CULTURAL DIFFERENCES IN EDUCATION: FOSTERING EQUALITY, CONNECTION, AND CRITICAL ENGAGEMENT IN THE MODERN CLASSROOM

Fun Man Fung^{a, b}, Hsiang-Lin Liu^c Yi-Hsin Liu^{*d}

^a*School of Chemistry, University College Dublin, Ireland*

UCD Geary Institute for Public Policy, University College Dublin, Ireland

^b*Department of Chemistry, Stanford University, California, United States.*

^c*Department of Physics, National Taiwan Normal University, Taipei, Taiwan*

^d*Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan*

**Corresponding author: yliu@ntnu.edu.tw*

Abstract

Cultural differences significantly shape educational practices and impact how students and teachers interact. This study explores the challenges and opportunities in addressing these differences, particularly focusing on equality, rapport building, and the influence of the virtual world on young learners. In many cultures, especially in Asian contexts, hierarchical structures dominate educational systems, often hindering open communication and mutual respect between students and teachers. Meanwhile, the younger generation's preference for the virtual world has created a disconnect, as they often fail to acquire meaningful knowledge or interpersonal skills from online interactions.

Our research incorporates innovative teaching tools, such as using two students performing a dance to simulate electron angular momentum around nuclei to visualize quantum concepts like wavefunction shapes, nodes, and quantum confinement energy. Additionally, we leverage Discord for private and group communications, enabling the sharing of public class information and addressing personal questions, fostering an inclusive and interactive learning environment. The study also implements peer evaluation strategies where students review and grade each other's video presentations. Full credits are awarded when expected and actual grades align, while significant divergences result in reduced credits, encouraging accountability and critical evaluation skills.

The findings highlight the importance of treating students as equal human beings, integrating creative tools like art and digital platforms to foster connection and understanding. Practical strategies for educators to build rapport and promote critical engagement in the classroom are discussed, with a specific focus on adapting these approaches to Asian educational systems. These strategies aim to modernize teaching practices and equip students with the skills needed to thrive in an interconnected and rapidly evolving world.

Keywords: Cultural Difference, Educational Equality, Quantum Chemistry Visualization, Rapport Building, Peer Evaluation Strategies

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CHEMICAL AUTOMATION: AN INNOVATIVE COURSE FOR THE AGE OF SMART CHEMISTRY

Changxu Lin^{a,b,*}, Zhaobin Chen^c, Ning Fang^{a,c}

^a State Key Laboratory of Physical Chemistry of Solid Surface, Xiamen, China.

^b College of Physical Science and Technology, Xiamen University, China.

^c College of Chemistry and Chemical Engineering, Xiamen University, China.

*Corresponding author: lincx@xmu.edu.cn

Abstract

In recent years, artificial intelligence has been applied to synthetic chemistry and has achieved a series of important results. The development of the interdisciplinary disciplines of chemistry and information technology, such as intelligent molecular manufacturing and chemical measurement, has put forward a new demand in quantity and quality for the training of talents with both knowledge of information technology and molecular science. In response to the needs of discipline personnel training, we improve the knowledge system of the new engineering major of chemical measurement, and newly set up chemical automation and supporting experiment courses. This report will briefly introduce the basic situation of the course.

The combination of courses has been offered in the spring semester of the academic year 22-23 and has received a high level of interest and participation from students. For theoretical courses, the latest automation, high throughput, algorithm and literature examples of chemistry, material synthesis and characterization are used to design lesson plans, and the course outline is designed according to the capability logic aspects of automation. In the auxiliary experiment course, I have a basic understanding of the basic working principle and functional module composition of the existing scheme using automation means in chemistry. In addition, the comprehensive application ability is cultivated in the large-scale operation. According to the needs of chemical experiments and corresponding automation needs, the technical ability is reasonably selected and matched, and the automation system is constructed to complete the corresponding experiments.

Keywords: Intelligent chemistry; Chemical automation; Experimental teaching; Comprehensive ability



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GENERATIVE AI ASSISTED DESIGN OF MACHINE LEARNING MODELS FOR POLYMER IDENTIFICATION AND SORTING IN UNDERGRADUATE LABS

Benji Fenech-Salerno^{a,*}, Rebecca L. Jones^a, Martin Holicky^b, Laura Patel^a.

^a*Department of Chemistry, Imperial College London, United Kingdom.*

^b*Matoha Instrumentation, London, United Kingdom.*

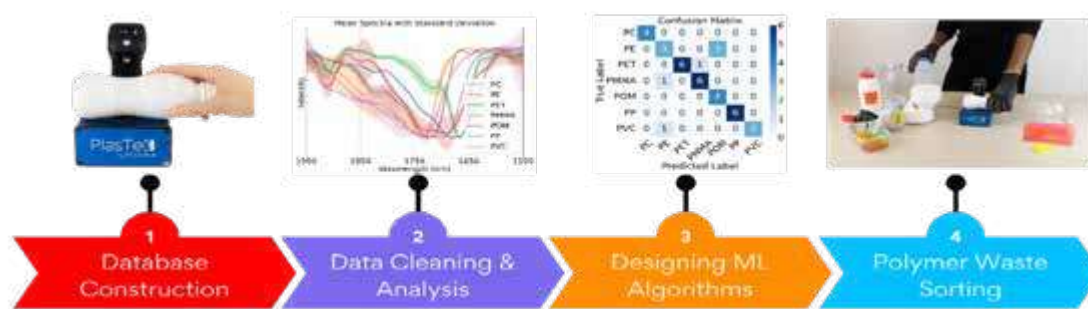
**Corresponding author: b.fenech-salerno@imperial.ac.uk*

Abstract

This presentation showcases an innovative laboratory framework that explores a critical bottleneck in polymer recycling: the accurate identification and characterisation of polymer waste.¹ Aligned with UN Sustainable Development Goal 12 for responsible consumption and production, the lab develops students' data science competencies within the context of real-world recycling challenges.²

The laboratory consists of four interconnected activities that progressively develop students' capabilities in both computational and experimental domains. Initially, students build a polymer reference database using near-infrared (NIR) spectroscopy (1), creating a foundation for their subsequent machine learning applications. They then engage in exploratory data analysis (2), applying statistical methods to assess spectral quality and identify outliers—skills fundamental to reliable data science and for reliable polymer identification in heterogeneous waste streams. All data analysis and data science tasks are conducted using Python, with generative AI enabling the construction of complex code that students evaluate, review, and manipulate according to their personal objectives and judgments. The third phase involves the development and optimisation of k-Nearest Neighbours (kNN) classification models (3), with students critically evaluating model performance through confusion matrices and classification metrics. Finally, students apply their optimised models to identify unknown polymer samples (4).

The presentation will also examine our scaffolded assessment strategy, which carefully sequences learning activities to build competencies progressively while providing appropriate support at each stage. Formative and summative evaluations reveal that students develop not only technical competencies in machine learning but also a deeper understanding of how data science tools can address sustainability challenges. Our final objective is to communicate key takeaways from this framework, which serves as a transferable model for embedding sustainability-focused data science education within chemistry curricula, equipping graduates with the necessary skills to address timely and complex societal challenges.



Keywords: data science, machine learning, generative AI, chemistry education, sustainability.

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ASSESSING STUDENTS' COLLABORATIVE LEARNING PROCESS IN IVR FOR LEARNING CHEMISTRY

**R. Bruno Hernandez-Alvarado^{a,*}, David F. Treagust^a, Mihye Won^b, Mauro Mocerino^a,
Chin-Chung Tsai^c, Roy Tasker^d**

^aCurtin University, Western Australia.

^bMonash University, Victoria, Australia.

^cNational Taiwan Normal University, Taipei, Taiwan.

^dWestern Sydney University, Australia

*Corresponding author: r.hernande@postgrad.curtin.edu.au

Abstract

Immersive virtual reality (iVR) has emerged as a promising tool in science education, offering unique affordances that can benefit collaborative learning. Research has shown that iVR can facilitate engagement, interaction, and conceptual understanding (Matovu et al., 2023). However, there is a need for a structural framework to assess the quality of collaboration in iVR environments. This study introduces a categorical framework designed to evaluate dyadic collaboration within an iVR-based chemistry learning experience. Nine student pairs participated in an iVR learning experience to learn about water crystallization and snowflake formation. Their interactions were systematically observed and analyzed to identify patterns of social engagement. The proposed framework differentiates collaboration quality into high, moderate, and low groups. These classifications are based on essential aspects of collaboration, including verbal responsiveness, peer assistance, and turn-taking (Meier et al., 2007), while also incorporating unique iVR affordances like gestures, body movements, and object manipulation. This research contributes to understanding collaborative dynamics in immersive environments, offering a methodological approach to assess collaborative learning in iVR. The proposed framework provides a structured approach to understanding how students interact with others inside iVR and highlights the role of iVR in shaping collaborative dynamics.

Keywords: Immersive virtual reality, collaborative learning, social interactions

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NI-CATALYSED CROSS-COUPPLINGS: UNDERGRADUATE-LED PRACTICAL INVESTIGATIONS

Ravi Singh^{a*}, Laura Patel^a

^a Department of Chemistry, South Kensington, Imperial College London, United Kingdom, SW7 2AZ

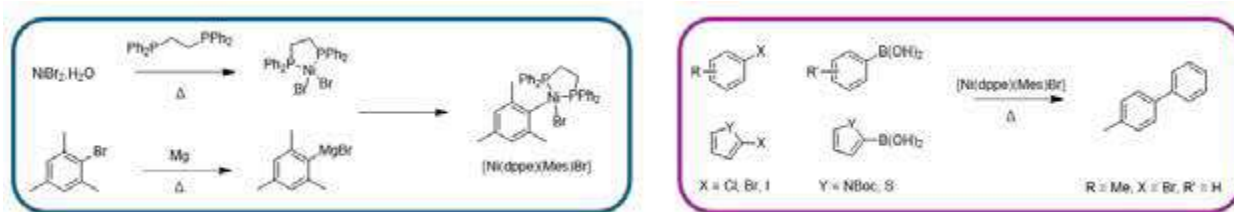
*Corresponding author: ravi.singh@imperial.ac.uk

Abstract

The use of palladium (Pd) for catalysis has become routine for the formation of C-C bonds which could not be achieved using ‘traditional’ organic chemistry. This has allowed transformations to be done in a catalytic manner, with a wide substrate scope, and was awarded the 2010 Nobel Prize in Chemistry.¹ The ‘Suzuki reaction’ is the second most popular reaction in industry owing to the ease of carbon-carbon bond formation.² Pd sources are now running low, owing to increased usage, and this has caused an increase in Pd costs. Efforts to move away from heavy metals, such as Pd, led to the idea of using nickel (Ni) instead.^{3,4}

Using this approach, we developed an inquiry-based lab practical which allows our third-year undergraduate students to explore this reaction using a Ni-catalyst.^{5,6} Students are each assigned a different reaction which they use as a basis for their investigation. Students have investigated steric effects and electron demand, across two different years, on the substrate scope. This practical also utilizes Nuclear Magnetic Resonance to monitor and estimate reaction progress in a semi-quantitative manner. From the results, we have been able to study a range of boronic acid-aryl halide cross-coupling reactions, including evidence of boronic acid homo-coupling. From this work, we have trained undergraduate students to prepare for research, through independent investigations, but have also learned about substrate scope and the effects on reaction rates.

Keywords: Ni-catalyzed cross-coupling chemistry, undergraduate laboratory experiments, inquiry-based practical, sustainability.



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EFFECTS OF ATTENTION REGULARITY IN CHEMISTRY ACHIEVEMENT, LEARNING INTERESTING, AND ATTITUDE AMONG HIGH SCHOOLS IN CHINA

Lai Xiaoqin, Chua Kah Heng*, Rose Amnah Abd Rauf

Faculty of Education, Universiti Malaya

**Corresponding author: chuakh@um.edu.my*

Abstract

In recent years, neuroscience has made significant progress in attention research¹. However, the development of educational neuroscience in China is still lagging behind compared to other developed countries, especially the application in classroom teaching, which is still in its infancy². This study investigated the feasibility and effectiveness of teaching chemistry based on students' attention regularity (AR). A quasi-experimental design was used to test 15-16-year-old high school students (56 in the experimental group and 54 in the control group) before and after a 12-week intervention, including chemistry achievement, interest in chemistry learning, and attitude toward chemistry learning. The results showed that teaching based on AR could significantly improve the students' chemistry achievement and learning interest and improve their learning attitude to some extent. This study provides Chinese high school chemistry teachers with empirical evidence for implementing attention-based teaching strategies and contributes to the promotional development of teachers.

Keywords: High school chemistry teaching, ar(attention regularity), non-chemistry students, chemistry achievement, learning interesting, attitude

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ENHANCING CHEMISTRY EDUCATION WITH AI-DRIVEN INTERACTIVE MODELS: A STUDY ON WADE'S RULE AND BORANE CLUSTERS

Mai Yan Yuen^{a*}

^a*Department of Chemistry, The University of Hong Kong.*

**Corresponding author: maiyan@hku.hk*

Abstract

Wade's rule is a fundamental concept in undergraduate inorganic chemistry, enabling students to predict the structures of borane clusters—such as closo, nido, or arachno—based on electron counts. Traditional instruction often relies on 2D and static diagrams, which many students find difficult to interpret, particularly when grappling with borane bonding and geometry. Interactive models offer a dynamic alternative, allowing students to visualize and manipulate structures, potentially enhancing engagement. However, unlike widely available organic chemistry models, effective tools for inorganic compounds like boranes are limited, the need for specialized resources are of great demand in the inorganic chemistry teaching and learning.

Recent advancements in artificial intelligence and AI-supported programming have streamlined this process. In this project, students utilize an AI-powered chatbot (Deepseek or Grok) and AI-assisted coding software (CURSOR or Visual Studio Code) to develop interactive borane models. Through this initiative, they acquire skills in AI interaction, foundational Python programming, and collaborative model-sharing with peers. Furthermore, by creating their own models, students deepen their understanding and build valuable computational competencies.

This approach has the potential to transform chemistry education by making complex concepts more accessible and interactive. It bridges traditional pedagogy with modern technology, equipping students with the skills required for contemporary scientific demands in a professional and effective manner.

Keywords: Wade's rule, AI-assisted programming, Interactive models, Chemical Education



SCIENCE COMMUNICATION IN CHEMISTRY: TRANSITIONING WITH GENERATIVE AI

Mohd Bakri Bakar^{a*}

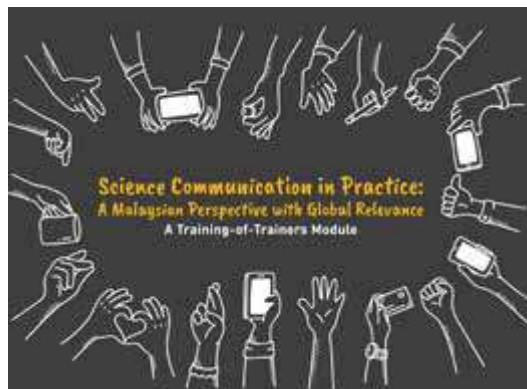
^a*Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia*

^{*}*Corresponding author: bakribakar@utm.my*

Abstract

The transition from pre-Generative Artificial Intelligence (pre-Gen AI) to post-Generative AI (post-Gen AI) has significantly impacted science communication, including the dissemination of chemistry knowledge to the public. Conventional science writing relied on manual research, structured storytelling and iterative refinement to ensure clarity and engagement. However, with the emergence of AI-driven tools, writing strategies have evolved, raising questions about their implications for scientific accuracy and public understanding. This presentation examines how science communication has evolved from pre-Gen AI to post-Gen AI, focusing on efficiency, accuracy and accessibility. It also explores the challenges of writing in Malay as a local language, including translation issues and terminology adaptation. A comparative analysis was conducted on science writing strategies before and after the integration of AI. The study draws from experiences in developing a science communication module published by the *Academy of Sciences Malaysia* (ASM) during the pre-Gen AI period and an ongoing revised module incorporating AI-assisted writing tools. Case studies from chemistry popular science articles, particularly those published via the ASM *esti.my* portal were analysed to assess changes. AI-assisted writing enhances efficiency and accessibility, allowing for faster content generation and simplified explanations of complex topics. However, challenges such as over-reliance on AI-generated text, potential inaccuracies and the need for human oversight remain critical. Writing in Malay presents additional challenges such as standardising terminology and ensuring scientific precision. The shift from pre-Gen AI to post-Gen AI has redefined science communication particularly in writing, offering both opportunities and challenges. While AI tools improve writing efficiency aiming to maintaining public trust in scientific information, their role should complement rather than replace human expertise.

Keywords: Popular Chemistry, Writing, Generative AI, Public engagement



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RETHINKING CHEMISTRY TRIPLET IN THE ERA OF GENERATIVE ARTIFICIAL INTELLIGENCE

GyeongGeon Lee^{a*}

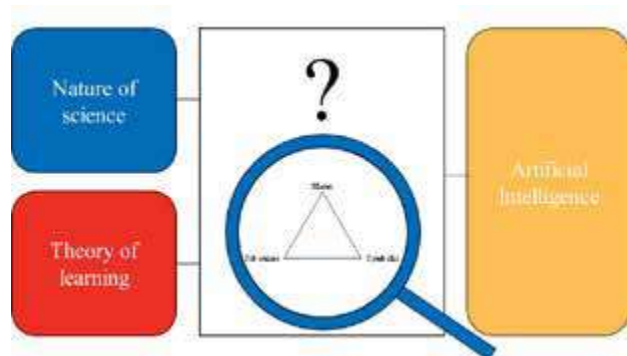
^aNational Institute of Education, Nanyang Technological University, Singapore

*Corresponding author: gyeonggeon.lee@nie.edu.sg

Abstract

Chemistry education has long been indebted to the chemistry triplet (CT) paradigm, initially proposed by A. H. Johnstone.¹ The triplet asserts that chemistry phenomena can be taught in terms of macro, micro, and symbolic representations and their relationship. Macro-scale representation denotes the level at which chemical phenomena are experienced (e.g., mass, density, pH, temperature), micro to the level at which models built from particles such as atoms, ions, and molecules, and symbolic to the level where signs (e.g., text, diagram, graph) are used to represent concepts and ideas². The CT approach has been considered a rationale for the need for multiple representations in chemistry education.² Also, scholars have clarified, elaborated, and extended the idea of CT for specific chemistry teaching and learning situations.³ However, as far as known to the author, there have been no works to re-position chemistry education around CT in the era of artificial intelligence (AI). In the 2020s, especially after the release of ChatGPT by OpenAI in November 2022, AI is taking the leading role of transforming educational landscapes worldwide. Further, 2024 Nobel Prizes for Chemistry (AlphaFold) and Physics (deep learning) call for renovations for what we learn (nature of science) and how we learn (theory of learning) in science education, respectively. In response, this study actively pursues the intersection of traditional chemistry education and cutting-edge AI studies, by revisiting the meanings of macro, sub-micro, and symbolic representations in CT. Particularly, multimodal AI models that are capable of processing text and image data simultaneously and generating resultant answers will be examined to rethink CT. The structuralist approach to language and reality will be the basis for the argument. Also, this study deliberates on how to center human and embodied nature for chemistry teaching and learning, even for the AI-shaped future.

Keywords: chemistry education, chemistry triplet, Johnstone's triangle, generative artificial intelligence, multiple representation



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MACHINE LEARNING FOR AUTOMATED SCORING AND TEXTBOOK ANALYSIS IN CHEMISTRY EDUCATION RESEARCH

Mei-Hung Chiu^{a,*}, Mao-Ren Zeng^b

^a*Professor Emerita, National Taiwan Normal University, Graduate Institute of Science Education*

^b*Research Associate, CREATE for STEM Institute, Michigan State University.*

**Corresponding author: mhchiu@gapps.ntnu.edu.tw*

Abstract

The rapid advancement of Artificial Intelligence (AI) offers opportunities and challenges for assessing students' responses to open-ended questions and analyzing textbooks. While machine learning (ML) has been widely applied in assessment research (e.g., Krajcik, 2021; Zhai, 2021), its use in evaluating Chinese-language responses remains limited (Wang et al., 2021). The implicit nature of Chinese expression and sentence structures makes automated analysis difficult, and many AI tools developed in Western contexts struggle with Chinese characters.

Textbooks play a crucial role in chemistry education, guiding both students and teachers. As computational techniques gain traction, ML methods like Latent Dirichlet Allocation (LDA) help analyze the coherence of chemistry content. AI-powered tools can reduce the labor-intensive nature of text analysis and offer new insights into chemistry education. This presentation explores two AI applications in chemistry education. First, we examine automated scoring of students' scientific explanations in Taiwan, involving 896 high school students. Responses were analyzed using the Claim-Evidence-Reasoning (CER) framework (McNeill & Krajcik, 2008). The ML-based scoring system showed satisfactory accuracy and Kappa values, demonstrating its potential for Chinese-language science assessments (Chiu & Zeng, 2024). Analytic analysis outperformed holistic evaluation in both accuracy and reliability.

Second, we applied Latent Dirichlet Allocation (LDA) to analyze six Taiwanese high school chemistry textbooks, identifying seven key topics. Topics such as Kinetics and Equilibrium slightly progressed in three textbooks, while chemical reactions and structure-function relationships appeared concurrently in two. These findings offer insights into content alignment with curriculum standards and instructional planning.

This presentation highlights how AI-based tools can enhance chemistry education, emphasizing educators' and researchers' competencies to integrate AI effectively.

Keywords: Artificial Intelligence, Machine Learning, LDA, automated scoring, textbook analysis, assessment

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THE ACS GLOBAL RECOGNITION PROGRAM AS A CATALYST TO FOSTERING CROSS BORDER COLLABORATIONS

Wasiu Lawal^a, Michelle Brooks^{a*}

^a*American Chemical Society*

**Corresponding Author: m_brooks@acs.org*

Abstract

History has shown repeatedly that for the global community to achieve lofty targets, such as the Sustainable Development Goals (SDGs), chemistry will have to play a leading role. Moreso, given the interconnected nature of the various issues the SDGs have set out to solve, scientific/educational collaborations across nations and continents will be vital towards achieving these goals.

The reality however suggests that for a multitude of reasons, scientists in developing countries, who tend to suffer the greatest consequences of the issues the being tackled by the SDGs, often find it difficult to establish meaningful partnerships with their counterparts in the developed world.

As the world's largest scientific organization, the American Chemical Society is strategically focused on supporting the global scientific community. One of the ways it does is through its Global Recognition Program, which evaluates and recognizes undergraduate Chemistry programs across the globe.

This presentation will discuss how the ACS Global Recognition Program aims to narrow the barriers between institutions on both sides of the economic divide through its guidelines and evaluation processes.

Keywords: Chemical Education, Accreditation, Guidelines, SDGs

CHEMICAL PHILATELY: THE WORLD OF CHEMISTRY ON POSTAGE STAMPS

Daniel Rabinovich^{a,*}

^a*The University of North Carolina at Greensboro*

*Corresponding author: Dan.Rabinovich@uncg.edu

Abstract

Postage stamps constitute a simple yet effective means of communication, often used by governments or postal authorities to inform the general public on a variety of topics, including historical events, tourist attractions, and national accomplishments in the arts. A surprisingly large number of stamps have also been issued to commemorate scientific discoveries or to honor well-known scientists.¹⁻³ This presentation will feature postage stamps pertaining to the history of chemistry, the discovery and sources of several chemical elements, the development of the periodic table, chemical formulas and structures, laboratory equipment, biochemistry, and various aspects of the chemical industry. Postage stamps, as we will demonstrate in this presentation, constitute a powerful tool to communicate science to non-scientists and to teach chemistry at all levels.

Keywords: Postage stamps, chemical philately, science communication, chemical education



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ARTIFICIAL INTELLIGENCE IN CHEMISTRY EDUCATION – WHERE ARE WE?

Jamie Khoo Zheng Yuan^{a,*}, Fun Man Fung^{b,*}, Jennifer Schwartz Poehlmann^c, Chin- Chung Tsai^d,
Yvonne Choo Shuen Lann^e, Fabian Hollinger^f, David Anzola^b, Chang Xu Lin^g

^aNational University of Singapore; ^bUniversity College Dublin; ^cStanford University; ^dNational Taiwan Normal University; ^eXiamen University Malaysia; ^fUniversity of Zurich; ^gXiamen University

*Corresponding author: jamie.kzy@u.nus.edu, funman.fung@ucd.ie

Abstract

Artificial intelligence (AI) capabilities stretch beyond chemistry research and are pivotal in shaping the solutions to many of society's concerns. The sustainable development goals, namely education, hold much anticipation of the future changes to pedagogical learning and teaching with the introduction of AI. Due to its high versatility and fast development, AI is expected to facilitate advancements in chemistry research. In the fields of drug discovery, integrated and big data, as well as laboratory automation, skillsets required to adapt quickly and efficiently with the pace of research growth have begun to evolve.

To project future directions and uses of AI in chemistry research, the history and its accomplishments were analysed. By looking at specific skillsets or ways of thinking and comparing them with the advancement of AI, vital skillsets for a future with AI in chemistry can be identified. This begets the importance of instilling such skillsets and honing the skill of adaptability in students to prepare them for a future fast-changing workplace. To best take advantage of the opportunities enabled by AI, chemistry education can focus on utilising AI in the classrooms for personalised learning experiences, pushing students to develop self-directed learning approaches to chemistry. The support for critical thinking and problem-solving skills also remains paramount in the future of AI, on which instructors can rely on AI to link broad ideas together, deepening students' comprehension of chemistry foundational knowledge. The importance of high-quality higher education is therefore vital to train chemists to develop forward-thinking mindsets.

We question then: Are chemistry students ready for the future of chemistry and AI? Based on the approach of Students as Partners (SaP), we share data from our review on how universities are equipping their undergraduates for a new future. Finally, we discuss our visions for the future as members of the chemistry community - the versatility of AI in advancing chemistry research and its impact on chemistry education.

Keywords: Chemistry Education, Artificial Intelligence, University Courses, Higher Education

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CHEMISTRY ON THE GO

**Hsien-Chang Kao^{a*}, Yu-Lin Lin^a, Ching-I Fan^a, Jia-Yu Shih^a, Heng-Cheng Kao^a,
Bo-Cheng Wang^b**

^a*Center of Science Education, Tamkang University, Tamsui, Taipei 25137, Taiwan.*

^b*Department of chemistry, Tamkang University, Tamsui, Taipei 25137, Taiwan.*

rogers.kao@mail.tku.edu.tw

Abstract

The United Nations General Assembly, with the backing from UNESCO, named 2011 the “International Year of Chemistry” (IYC2011) under the theme: “Chemistry - our lives, our future.” Chemistry On the Go is one of very few projects that is still ongoing and making chemistry available to as many students as possible, especially in under-served areas around Taiwan.

The idea was to convert the two box trucks to create two separate programs that can, when needed, work in tandem and go to junior and senior high schools in every county and city in Taiwan. Exterior of the box trucks is painted with deliberate and colourful design to deliver chemistry information. The Mobile Lab is a 3.5-ton box truck converted into a laboratory-like stage. It is equipped with all the necessary chemicals and supplies to introduce chemistry through magic shows, historical stories, mini-lectures, demonstrations, and hands-on experiments. Programs in the Mobile Lab were designed to be fun, interesting and colourful to enhance the curiosity of students. The Analyst Lab focuses on bringing analytical experiments about food and the environment to the public and students. This allows them to get a glimpse into their future.

Since IYC 2011, Chemistry On the Go has travelled more than 150,000 KM all around Taiwan, hosting 800 events in schools in various areas. Over 100,000 students have participated in these activities.

Support from the government and industry collaborations fund the programs and the manpower. Industry employees volunteer for some activities and provide students with opportunities to interact face-to-face with professionals while allowing the industry to better understand the challenges faced by schools in the surrounding areas. Therefore, Chemistry On the Go can be seen as a model that integrates science education with social responsibility while promoting public understanding of chemistry.

Keywords: International Year of Chemistry 2011, Mobile Lab, Analyst Lab, Corporate Social Responsibility, University Social Responsibility



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INTEGRATING DESIGN THINKING PROCESS, SUSTAINABILITY, AND A LIFE SIMULATION GAME IN DESIGNING A CHEMISTRY LABORATORY ROOM

Ralph Lauren M. Alomia^{a,*}, Hazel Joyce M. Ramirez^b, Elmer Rico E. Mojica^{a,c}

^a*Institute of Chemistry, College of Arts and Sciences, UP Los Baños, College, Laguna, Philippines.*

^b*College of Education, UP Diliman, Quezon City, Philippines.*

^c*Pace University, New York, USA.*

**Corresponding author: rmalomia@up.edu.ph*

Abstract

Chemistry classrooms are pivotal spaces for fostering active and meaningful learning. Yet, many remain predominantly content-heavy, offering limited opportunities for students to tackle real-world issues. Incorporating design thinking into chemistry education could address this gap by enabling students to engage in human-centered and creative problem-solving strategies while applying chemistry lessons. In this light, this research explored the integration of design thinking and sustainability principles in a class project where students were tasked to design a chemistry research laboratory room. The research participants were 43 BS Chemistry and BS Agricultural Chemistry students. As part of the process, the students utilized the SIMS 4™ (EA Games) game, which was originally designed as a life simulation game but was repurposed to be an educational technology tool. Particularly, the students worked in pairs to design chemistry laboratory room where they gathered and integrated insights from different stakeholders' perspectives, chemistry concepts, and sustainable practices such as chemical waste management. Research findings showed that students perceived that this teaching strategy enhanced their learning engagement and allowed them to further develop their critical thinking, creativity, and interpersonal skills. Additionally, this pedagogical approach fostered a deeper appreciation and understanding of chemistry concepts. This research offers essential implications for future practice and research direction by highlighting the synergy of design thinking, sustainability principles, and educational technology that allows students to develop 21st-century skills and promote sustainability practices and solutions.

Keywords: Design Thinking, Chemistry Laboratory Design, SIMS 4, Sustainability, Life Simulation Game

INTEGRATING SYSTEMS THINKING INTO CHEMISTRY EDUCATION TO ENHANCING PRE-SERVICE TEACHERS' CLIMATE CHANGE INSTRUCTION

Chua Kah Heng

Department of Mathematics and Science Education, Faculty of Education

University Malaya

**Corresponding author: chuakh@um.edu.my*

Abstract

Climate change is a complex global challenge that requires interdisciplinary understanding, yet chemistry education often addresses it through isolated concepts rather than interconnected systems. This project explores how systems thinking can enhance chemistry education by engaging pre-service chemistry teachers in developing systems thinking skills to teach climate change more effectively, linking chemical concepts with the Sustainable Development Goals. The entire project spanned 14 weeks using a One-Group Pretest-Posttest Design. Through the project, pre-service chemistry teachers undergo a structured four-phase approach: (1) an introduction to systems thinking and climate change, (2) examining climate science through a systems perspective, (3) creating systems-thinking lesson plans for teaching climate change concepts, and (4) evaluating and refining their lesson plans through peer-reviewed micro-teaching sessions. During the evaluation, the focus is on pre-service chemistry teachers' capacity to demonstrate chemical interconnectedness in climate systems, develop aligned instructional materials, and foster critical thinking about climate solutions. Statistical results showed a significant difference in pre-service chemistry teachers' knowledge of climate change and systems thinking skills. This project advances chemistry education by demonstrating how systems approaches can transform the teaching of climate-related chemical concepts, preparing educators to develop students' systems literacy for addressing this urgent global issue.

Keywords: System Thinking, Climate Change, Pre-Service Chemistry Teacher, Sustainable Development Goals

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AN INQUIRY-BASED LEARNING ACTIVITY OF OPTICAL ROTATION USING A 3D-PRINTED POLARIMETER

K. C. WONG^{a,*}, E. W. IP^a, W. H. Ng^a

^a*Department of Pharmacology and Pharmacy, The University of Hong Kong, Hong Kong Special Administrative Region, 999077, People of Republic China.*

**Corresponding author: kcwong47@hku.hk*

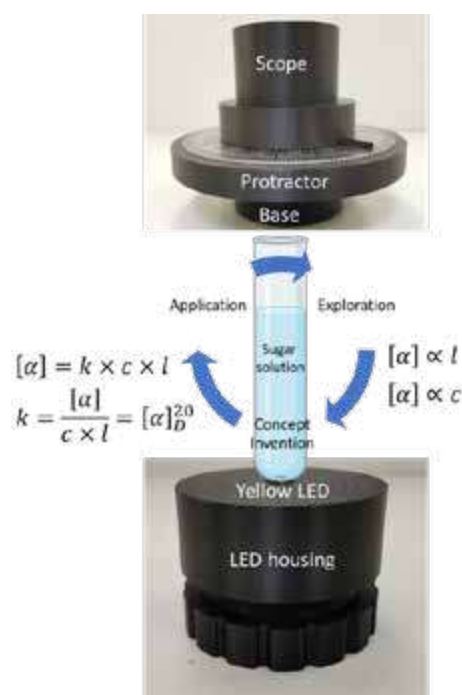
Abstract

This poster presents an innovative organic chemistry lab activity centered on optical rotation, using an inquiry-based learning approach with a 3D-printed polarimeter. Students performed hands-on experiments to measure the optical rotation of sugar solutions, exploring how concentration and path length affect rotation values. Guided by instructors, they derived the equation relating absolute rotation to concentration and path length, identifying the specific rotation constant.

Students then used this equation and the polarimeter to determine specific rotation values of various sugar solutions. The activity culminated in analyzing commercial sweeteners like honey and agave syrup, where students measured optical rotation to deduce the principal sugars and their ratios.

This educational activity deepened students' understanding of optical rotation and honed their analytical skills. Detailed procedures and student feedback will be presented in this poster.

Keywords: Inquiry-based Learning, Organic chemistry, Optical Rotation, 3D-printing



TRENDS IN THE OUTCOMES OF STUDYING CHEMISTRY DISCIPLINES AT A UNIVERSITY WITH A NON-CHEMISTRY MAJOR

Alena Vollmannová^a, Judita Lidiková^{a*}, Natália Čeryová^a, Janette Musilová^a

^a*Institute of Food Sciences, Faculty of Biotechnology and Food Sciences, Slovak University of Agriculture in Nitra*

^{*}*Corresponding author: judita.lidikova@uniag.sk*

Abstract

Chemistry is a fundamental scientific discipline with wide-ranging applications in medicine, agriculture, materials science, and energy. A foundational understanding of its core principles is essential even for students in non-chemistry fields. However, many students outside of chemistry-related majors often find the subject challenging and struggle to see its relevance to their studies.

This study analyzes long-term trends in student performance in chemistry-related courses at the Slovak University of Agriculture in Nitra, Slovak Republic. Specifically, we examine student outcomes in Inorganic Chemistry, Organic Chemistry, Analytical Chemistry, and Food Chemistry over the past 15 years, focusing on students enrolled in Food Sciences and Biology programs.

Despite a significant decline in enrollment, with student participation in chemistry courses decreasing by an average of 62.3%, the overall success rate has not shown a statistically significant decline ($p < 0.05$), decreasing by only 4.67% on average.

The findings suggest that while fewer students enroll in chemistry courses, those who do are likely to complete them successfully, possibly due to improved pedagogical strategies and stronger motivation among remaining students. These insights highlight the need for further adaptation of teaching methods to maintain and enhance learning outcomes in chemistry education for Food Science and Biology students.

Keywords: chemistry, education, success rate

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BRINGING A CHEMICAL SCIENTIST'S PERSPECTIVE AND EXPERTISE TO POLICY SPACES IN THE UNITED STATES

Annabelle T. Lolinco^{a,b,*}

^a*American Association for the Advancement of Science – Science & Technology Policy Fellowship*

^b*American Chemical Society – Public Policy Fellowship*

^{*}*Corresponding author: lolinco.belle@gmail.com*

Abstract

Science and technology innovation continue to shape modern society at an increasingly rapid pace, impacting all facets of life, from economic growth to public health. That same scientific expertise and training has value in shaping evidence-informed decision-making. In the United States, scientists have several different opportunities to get involved in policy spaces, whether it be working in traditional institutions such as academia or industry, or other avenues such as through government, think tanks, non-profits, trade associations, and so on. To expand on one such opportunity, working in the U.S. government can also include bringing scientific training to the legislative branch. The American Association for the Advancement of Science, working alongside other scientific societies, operates the Science and Technology Policy Fellowship (STPF). Dr. Lolinco shares how she navigated her chemical education and professional development opportunities to include work within science policy, advocacy, communication, and diplomacy spaces. Additionally, she will discuss her fellowship experience, highlighting what she brings and, in turn, how science has a place in policymaking. This presentation will include potential opportunities for scientists, at any career stage, to think about ways they too can use their scientific knowledge to influence decision-making processes.

Keywords: career exploration, experiential learning, science policy, diverse pathways, professional development

INTEGRATING EDUCATION FOR SUSTAINABLE DEVELOPMENT INTO A CHEMISTRY-CENTERED STEM INITIATIVE: A CASE STUDY OF THE ‘JOURNEY OF PLASTIC’ IN VIETNAM

Pham Xuan Phu^{a*}

^aBen Tre High School for The Gifted

*Corresponding author: xuanphubt@gmail.com

Abstract

The STEM education model is currently considered as an appropriate approach for Vietnam’s novel General Education Program, enabling students to explore and apply scientific knowledge to address real-world problems. Specifically, education for a sustainable future incorporates the environmental, economic, and social aspects into teaching and learning. Therefore, the integration of STEM education with sustainable development principles and chemistry should be prioritized to enhance educational outcomes. This study introduces a sustainable development model combining the STEM Chemistry course with expert and teacher consultations through the “Journey of Plastic” project on the topic of polymers in the 12th-grade Chemistry curriculum which was implemented by students from 12 Physics class at Ben Tre High School for The Gifted in southern Vietnam. Students engaged in this project undertake a range of activities, including a polymer exhibition, a slime-making workshop, and the Plastic for Trees program. Utilizing the collected plastic, students demonstrate proficiency in designing an infographic illustrating the plastic life cycle, repurposing materials into functional products, and developing bioplastics. Consequently, the project has gained widespread recognition across social media platforms, school newsletters, and Youth Union meetings in Ben Tre province. Findings from pedagogical experiments conducted on 30 students indicate that this integration positively influences their awareness and attitudes toward sustainable development issues while also fostering greater interest in Chemistry. Simultaneously, the research proposes recommendations for project implementation that correspond to students’ academic levels.

Keywords: Education for Sustainable Development, STEM Chemistry, STEM education model, Polymers, Plastic life cycle, Bioplastics.

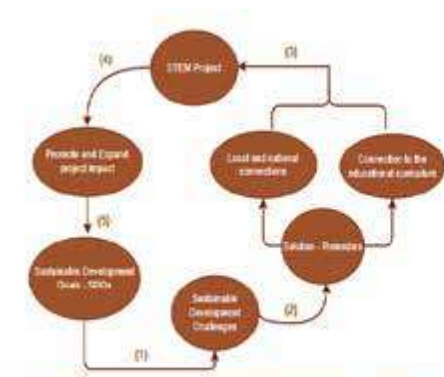


Figure 1: The Sustainable Education and STEM Integration Process – Addressing Sustainable Development through Local, National, and Educational Connections.

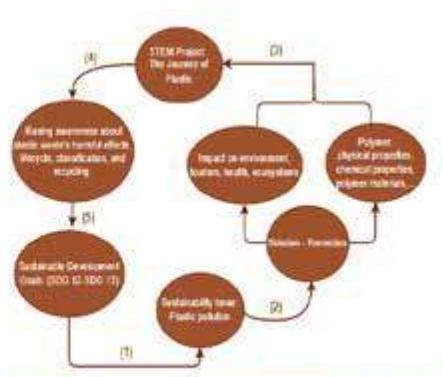


Figure 2: The Sustainable Education and STEM Integration Process – Polymer topic

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FOSTERING SUSTAINABLE DEVELOPMENT AWARENESS THROUGH SYSTEMS THINKING-INFORMED SMALL-SCALE CHEMISTRY EXPERIMENTS IN HIGH SCHOOL EDUCATION

Thanh Vinh Le^{a,*}

^a*Lawrence S. Ting school.*

**Corresponding author: thanhvinhchem@gmail.com*

Abstract

The integration of sustainable development principles into high school education is crucial for cultivating environmentally responsible citizens. This research proposes a pedagogical approach that utilizes systems thinking to structure and contextualize small-scale experiments, enabling students to explore the interconnectedness of chemical processes, resource utilization, and environmental impact. A series of small-scale experiments, designed through a systems lens, were developed, focusing on principles such as waste reduction, and green chemistry. The research employs a mixed-methods approach, combining quantitative assessments of students' conceptual understanding and qualitative analyses of their problem-solving processes and reflective narratives. Pre- and post-intervention surveys and focus group discussions were used to evaluate changes in students' awareness and perceptions of sustainable development. Preliminary findings indicate that the systems thinking-informed small-scale experiments significantly enhanced students' ability to analyze complex environmental issues, understand the implications of chemical practices, and recognize their roles in promoting sustainability. 91% of students demonstrate a deeper understanding of concepts related to sustainable development and 63.6% of students come up with concrete measures to take action for the environment. This study underscores the potential of integrating systems thinking and small-scale chemistry to foster a deeper understanding of sustainable development among high school students, providing a model for future curriculum development and pedagogical innovation.

Keywords: Sustainable Development Awareness, Small-Scale Chemistry, Systems Thinking

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CULTIVATING SYSTEMS THINKING USING THE SUSTAINABILITY COMPASS: A CASE STUDY ON GRADE 12 CHEMISTRY TOPICS IN VIETNAM EDUCATION CURRICULUM

Tai Nguyen Minh^{a,*}

^aNguyen Cong Tru High School, Ho Chi Minh City, Vietnam

*Corresponding author: minhtaipg@gmail.com

Abstract

This study aims to examine the effectiveness of the Sustainability Compass in strengthening students' systems thinking skills in the context of complex environmental challenges. The Sustainability Compass framework, which consists of four quadrants: Nature, Economy, Society, and Well-being, was used to guide the 12th graders in analyzing environmental issues like *forest degradation* and *plastic pollution* (also referred to as 'white pollution') as well as *metal recycling*. The pedagogical results observed in 41 students suggest that the Sustainability Compass captures the multidimensionality of these problems, both linked and systematically. Looking through the lens of each quadrant and the relationship amongst them allows students to understand these phenomena contextually, moving away from oversimplified linear explanations. This process transforms these students from passive observers to active and engaged participants whereby they can problematize the connection between the social, environmental, economic, and even individual spheres. Such systems thinking transforms how students recognize *leverage points* and *construct environmentally sustainable solutions* that encompass various facets of the issues, thus making them more prepared to face real issues of sustainability.

Keywords: sustainability compass, systems thinking skills, leverage points, environmentally sustainable solutions, chemistry education

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FOSTERING SYSTEMS THINKING IN HIGH SCHOOL CHEMISTRY THROUGH CARD-BASED LEARNING: A CASE STUDY IN VIETNAM

Tuan Nguyen Minh^{a,*}, Tai Nguyen Minh^b, Nhu Do Hien^c

^aHanoi National University of Education, Hanoi City, Vietnam

^bNguyen Cong Tru High School, Ho Chi Minh City, Vietnam

^cNguyen Thi Minh Khai High School, Ho Chi Minh City, Vietnam

*Corresponding author: edu.tuannm@gmail.com

Abstract

Developing systems thinking skills in chemistry education is essential for enabling students to analyze complex chemical phenomena and their broader implications. Systems thinking allows learners to connect chemical concepts with real-world contexts, fostering deeper conceptual understanding. However, integrating systems thinking into high school chemistry remains a pedagogical challenge, particularly in Vietnam. This study aims to foster systems thinking in high school chemistry through card-based learning, providing an innovative approach to teaching chemistry using active learning strategies. A classroom intervention was conducted with high school students in Vietnam, where card-based learning was integrated into lessons following the educational framework for teaching chemistry using a systems thinking approach¹. Students used interactive learning cards to explore system components, analyze interactions, and identify feedback loops within chemical systems. Data collection included self-assessment questionnaires and analysis of student learning artifacts, such as conceptual diagrams and written explanations, to evaluate their development of systems thinking skills². Preliminary findings indicate that students demonstrated improvements in key indicators of systems thinking when engaging with card-based learning. This study provides evidence that card-based learning is a promising approach to fostering systems thinking in high school chemistry. The integration of systems thinking frameworks with student-centered learning activities enhances chemistry instruction and may be adapted to broader educational contexts.

Keywords: Systems thinking, chemistry education, card-based learning, Vietnam



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APPLYING SYSTEMS THINKING TO DEVELOP A SUSTAINABLE HEAVY METAL WASTEWATER TREATMENT PROCESS

Nguyen Thi Thanh Phuc^{a,b,*}, Tran Thao Phuong^b, Tran Nguyen Hoang Long^b,
Mai Thi Phuong^c

^aHUTECH university, Ho Chi Minh city, Vietnam.

^bNguyen Cong Tru High school, Ho Chi Minh city, Vietnam.

^cVietnam Institute of Educational Sciences.

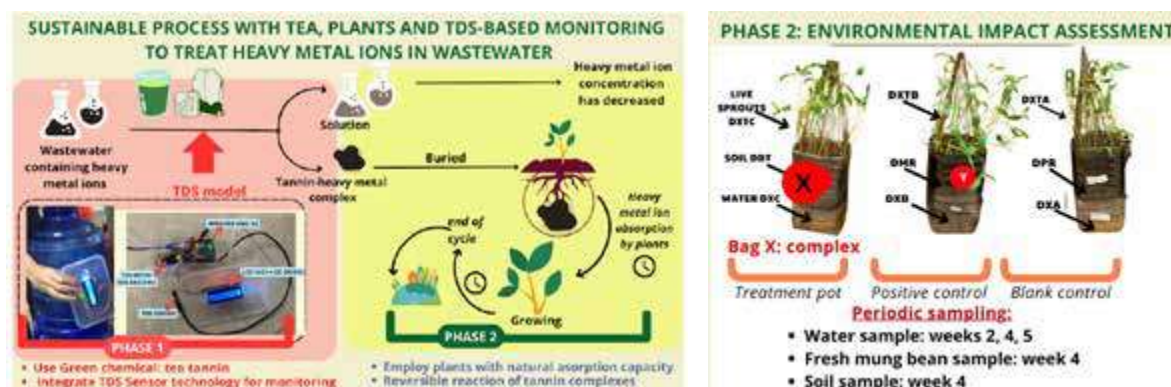
*Corresponding author: ntt.phuc@hutech.edu.vn

Abstract

Heavy metal wastewater from laboratories, particularly Cu^{2+} and Fe^{3+} , poses environmental risks, yet conventional treatments focus on precipitation without addressing long-term disposal. Applying Systems Thinking in Chemistry for Sustainability (STCS), this study aim to (1) develop a sustainable wastewater treatment process using tea tannin and plants, (2) design a TDS sensor system for monitoring treatment effectiveness, (3) evaluate environmental impacts when tannin-metal complexes are buried in soil, and (4) enhance students' systems thinking skills in sustainable chemistry education. The study utilized the Plan-Implement-Assess framework from SaSTICE, in two phases: Phase 1: Students treated wastewater with tea tannin and used an Arduino-based TDS sensor to measure Cu^{2+} and Fe^{3+} concentrations before and after treatment. Phase 2: Tannin-metal complexes were buried in soil with control setups. Students monitored metal ion release in soil, leaching into water, and plant uptake.

Tea tannin effectively removed 93.9% of Cu^{2+} and 91.5% of Fe^{3+} from wastewater, reducing total dissolved solids (TDS) from 6000 ppm to 1000 ppm, which validated the accuracy of the Arduino-based TDS sensor. When tannin-metal complexes were buried in soil, the release of Cu^{2+} was significantly lower (92.7 mg/kg) compared to the control (269 mg/kg), and Cu^{2+} concentrations in water remained low (<0.05 mg/L by week 4). However, Fe^{3+} exhibited increased leaching, reaching 4.49 mg/L by week 4. Plant uptake of Fe^{3+} improved, increasing from 17.07 mg/kg to 48.59 mg/kg, demonstrating the potential for controlled metal release and phytoremediation. By applying systems thinking, students analyzed feedback loops, optimized metal retention and release, and developed a cost-effective, eco-friendly wastewater treatment model. This research integrates green chemistry and STEM education, offering a scalable and sustainable solution for school wastewater treatment.

Keywords: Systems Thinking, Green Chemistry, Wastewater Treatment, TDS Sensor, Phytoremediation



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“CHEMTASTIC BIODIVERSITY!” TEACHING AND LEARNING CHEMISTRY FROM, WITH AND FOR BIODIVERSITY

Tejas Joshi

Independent Educationist and Former Humboldt Fellow, India.

**Corresponding author: tejasoldifluff@gmail.com*

Abstract

This presentation showcases “Chemtastic Biodiversity!”, a hybrid print-web based educational resource designed for chemistry teachers to introduce the domains of biodiversity, sustainability and ecological stewardship in their practice. Originating in the much-emphasized goal of chemistry education leading to a sustainable future, this resource is a lucid, creative attempt to devise a co-curricular learning tool towards bridging the conventionally separately taught disciplines of chemistry, biology and environmental education.

Designed with guided-inquiry and constructivist principles aimed at fostering an array of competences demanded by education for sustainable development (ESD) models, this resource is essentially a set of visual cards, viz. an alphabet of purposively selected floral-faunal species or ecosystems which “unfold” into varied chemical, human, ecological contexts through anecdotal snippets of information. A salient feature is the form factor of the cards – that makes the most of the print medium through the victorian fold puzzle. This mechanism not only heightens the scaffolding and tactile experience, but also offers designated spaces to strategically place contexts, graphics and keywords.

Each card demonstrates the rich spectrum of contextualized chemistry concepts that could be learned through biodiversity as also their interwovenness with broader ecosystems and global challenges. Cumulatively, the alphabet comes together in symbolizing how this chemistry knowledge can be responsibly deployed for protecting our planet and why it is paramount in achieving the United Nations’ Sustainable Development Goals. Tactical questions, ideas for further exploration as well as provisions of small spaces for even penning one’s own contexts pave the way to independent learner-led project opportunities in classroom and informal settings.

The poster offers a hands-on experience with the actual material, alongside providing a summary of the conceptual orientation, structure and overview of the chemical contexts underpinning the card-set.

Keywords: Chemistry education, chemistry for sustainability, ecological stewardship, biodiversity conservation, education for sustainable development (ESD)

THE EFFECT OF CHEMICAL EXPERIMENTS ON LEARNING SATISFACTION OF 10-GRADE STUDENTS

Son Chanthirit

New Generation Pedagogical Research Center, National Institute of Education

**Corresponding author: son.chanthirit.hs@moeys.gov.kh*

Abstract

Chemistry is a challenging subject for students, who struggle to understand its complex concepts without experiments. Teachers often fail to conduct these experiments due to some reasons like time constraints, lack of materials, and inadequate support from the school. The research aims to understand whether chemical experiments affect on grade 10 students' learning satisfaction and students' perspective on Chemistry at Hun Sen Boribo High School. To achieve these aims, Mixed-Methods Explanatory Sequential Research Design, which incorporates two distinct phases: a quantitative phase followed by a qualitative phase was employed. In the first semester of the academic year, experimental and control groups were arranged by the researcher with the help of the school administrators and the chemistry teacher who was teaching in those groups. Forty-nine students in the experimental group were taught in the class where the teacher conducted experiments. While forty-eight students in the control group were taught in the classroom where there were not any chemical experiments. Pre-test and post-test were conducted in both groups to check whether there was a statistical difference in their learning motivation. To deepen the understanding of students' satisfaction with chemistry subject in experimental and control groups, eleven students from the two groups were selected to participate in the interview. The findings from the pre-test and post-test indicate no statistically significant difference ($p > .05$) in both control and experimental groups. In addition, the findings from the post-test on both groups revealed no statistically significant difference either ($p > .05$). Therefore, students did not show any difference in learning satisfaction whether or not chemical experiments were conducted by their teacher. Even so, students in both groups suggest their chemistry teacher conduct chemical experiments, bring supplementary materials or interesting lessons, and customize in-class learning to be more engaging.

Keywords: Learning satisfaction, Chemical experiments, Effect

ENHANCING STEREOCHEMISTRY EDUCATION THROUGH INQUIRY-BASED LEARNING AND CONCRETE MOLECULAR MODELS

Kong-Ching WONG^{a,*}, Ignatius IP^a, Elvis Wang Hei NG^a,

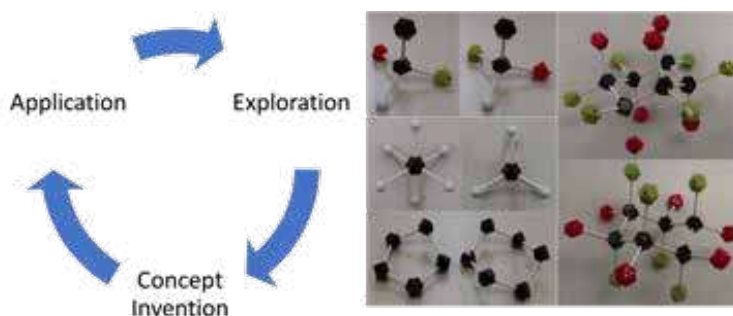
^a*Department of Pharmacology and Pharmacy, The University of Hong Kong, Hong Kong Special Administrative Region, 999077, People of Republic China.*

**Corresponding author: kwong47@hku.hk*

Abstract

Stereochemistry is a foundational yet challenging component of pharmacy education, often hindered by its reliance on complex spatial reasoning. To address these difficulties, this study introduces an innovative, inquiry-based learning activity that integrates concrete molecular models to enhance students' understanding of stereochemistry. Structured around a three-phase learning cycle—exploration, concept invention, and application—the activity was scaffolded by mini-lectures and conducted in small groups. Students actively constructed and analyzed 3D molecular models of organic compound isomers, enabling them to formulate definitions and rules for various types of isomerism. The use of tangible models reduced cognitive load by externalizing spatial processes, while also providing kinesthetic and proprioceptive stimulation, which are critical for spatial learning. Feedback from participants highlighted the activity's effectiveness, with students emphasizing the benefits of hands-on models and collaborative group interactions. This approach not only made stereochemistry more engaging but also more accessible, fostering a deeper understanding of the subject. By combining inquiry-based learning with tactile and visual aids, this method offers a promising strategy to support students in mastering the intricate spatial relationships essential to stereochemistry. The positive reception and demonstrated potential for improved learning outcomes suggest that this innovative approach could be a valuable addition to pharmacy and chemistry education curricula.

Keywords: Hands-On Learning, Inquiry-Based, Stereochemistry, Organic chemistry, Conformational analysis



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BUILDING CARD SET FOR CHEMICAL EDUCATION

Israel López^{a,*}, Arlethe Y. Aguilar-Villarreal^a, Eugenio Hernández-Fernández^a, Alejandro Vázquez^a, Carlos Puente^b

^aUniversidad Autónoma de Nuevo León (UANL), Facultad de Ciencias Químicas (FCQ), San Nicolas de los Garza, Nuevo Leon, Mexico

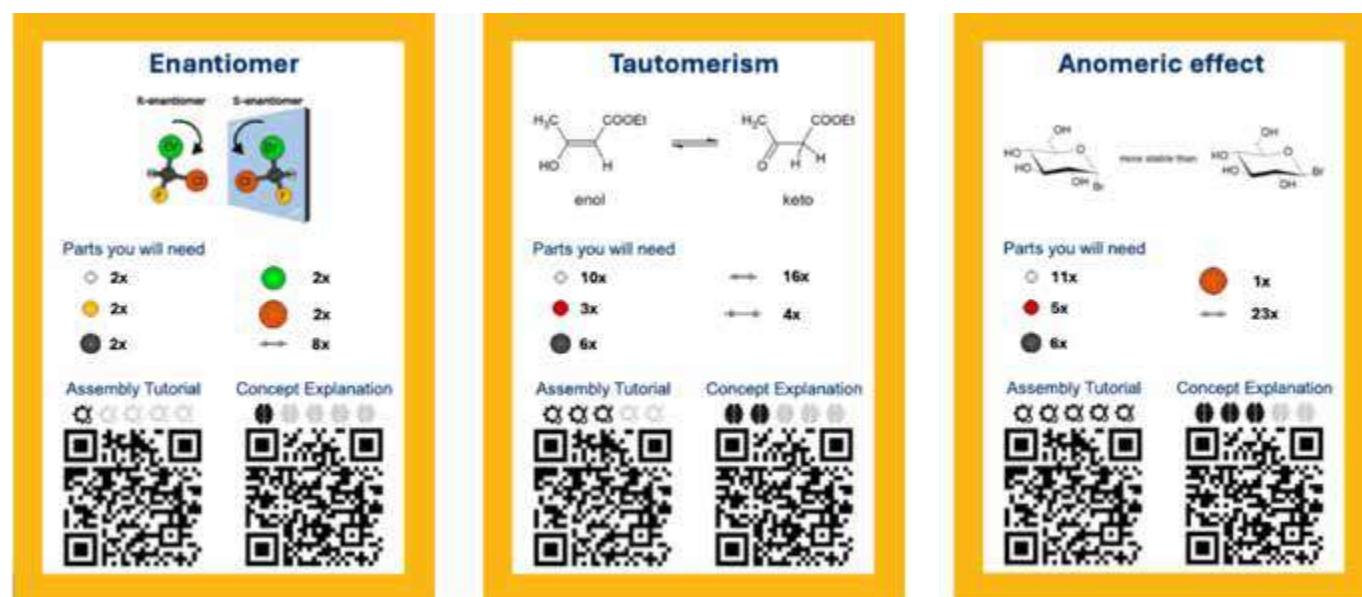
^bSchool of Engineering and Sciences, Tecnológico de Monterrey, Monterrey, Nuevo Leon, Mexico

*Corresponding author: israel.lopezhr@uanl.edu.mx

Abstract

Understanding some concepts in Chemistry can be difficult without a visual guide that allows any student to illustrate a specific example. There is a wide variety of construction models for molecules¹ and crystal structures², which have different assembly methods and materials. These building models themselves do not allow autonomous or semi-autonomous learning; however, multimedia content can complement the information required by any self-learner. In this proposal, a deck of cards serves as the link between the multimedia content and the building model, with each card addressing a chemical concept³⁻⁵. These cards present a simple representation of a chemical concept, as well as the type and number of parts required for its assembly. Two QR codes are included on the cards: the first is an assembly tutorial video, and the second corresponds to an explanation video of the chemical concept. The associated difficulty level for each model is indicated on both QR codes.

Keywords: chemical education, card set, building model kit, multimedia, self-learning



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CULTIVATING SCIENTIFIC INQUIRY IN YOUTH THROUGH HIGH SCHOOL RESEARCH CONFERENCES

Rameshwar Adhikari¹, Om Prakash Basyal¹, Jaya Ram Ghimire¹, Elina Maharjan¹, Rajesh Pandit^{1,2*}, Prasamsha Panta¹, Num Kant Parajuli¹, Manish Man Shrestha¹, Nelson Rai¹, Umesh Subedi¹, Dikshya Suwal¹ Umesh Thapa¹

¹*Nepal Polymer Institute (NPI), P. O. Box 24411, Kathmandu, Nepal*

²*Tri-Chandra Multiple Campus, Tribhuvan University, Kathmandu, Nepal*

**Corresponding e-mail: panditrajesh02@gmail.com*

Abstract

Over the past decade, the Nepal Polymer Institute, the national adhering organization of IUPAC in Nepal, has been organizing annual Young Scientists Summits (YSS) that bring together high school and senior high school students, their teachers, and university mentors to engage in hands-on scientific research. These summits span a wide range of disciplines, including chemistry, biology, environmental science, physics, mathematics, engineering, robotics, and artificial intelligence. The conferences have served as vibrant platforms where students present their research projects, often mentored or co-mentored by university faculty, research scholars, or graduate students at the Master's and Ph.D. levels. Through this process, students gain early exposure to scientific inquiry, and many students even learn the art of scientific writing, with opportunities to publish their work in peer-reviewed journals. Our experience over the years has shown that such initiatives not only inspire students by nurturing a research mindset from a young age but also empower teachers with new skills and perspectives that enrich their professional journey. High school students have consistently demonstrated remarkable energy and enthusiasm for research. Beyond academic growth, this early engagement fosters creativity, critical thinking, and problem-solving, skills that are foundational to innovation, entrepreneurship, and broader societal impact.

This presentation will share the outcomes, lessons learned, and future potential of this model as a scalable and replicable framework for bridging schools and universities. It aims to highlight how early research exposure, particularly in chemistry and related sciences aligned with global needs, can empower the next generation of scientists, innovators, and changemakers. Young scientists conferences like YSS can serve as powerful platforms for cultivating a research culture from an early age. However, to ensure their sustainability and broader reach, it is essential for local governments and national academies to recognize these initiatives as valuable assets and to invest in them. Supporting young scientists today is an investment in a more innovative, equitable, and sustainable future for all.

TECHNOLOGY ENHANCED EXPERIMENT BASED LEARNING IN SURFACE CHEMISTRY LECTURES

Chin Swee Yee¹, Teo Chian Ying¹, Vasudeva Rao Avupati¹

¹*School of Pharmacy, International Medical University, Bukit Jalil, Kuala Lumpur 57000, Malaysia.*

**Corresponding author: chinsweeyee@gmail.com*

Abstract

The incorporation of experimental demonstrations holds significant value in the teaching of chemistry, biology, and physics across all educational levels. These practical experiences play a crucial role in enhancing understanding within these challenging yet vital disciplines. Consequently, there is a recognized need for university-level instructors to seamlessly integrate insightful experiments and demonstrations into their lectures.

The use of engaging experiments, complemented by animated videos during lectures, serves multiple purposes. It can serve as a means to introduce novel concepts or to elucidate intricate aspects of subjects that students often find challenging. By presenting convincing results, these experiments empower students to take ownership of new ideas, providing a scaffold for their learning process.

This study aims to develop an innovative lecture format that seamlessly integrates entertaining experiments with animated videos, fostering an active learning environment. By combining interactive sessions with on-site fun experiments, this approach stands out as more engaging and enjoyable compared to conventional lecture methods. The overarching goal of this study is to enhance the overall learning experience and stimulate students' interest in the subject matter.

The impact of this research lies in promoting dynamic and interactive sessions that captivate students, encouraging a deeper connection with the material. This approach aligns with the current era of learning and is particularly well-suited for online education. Moreover, the incorporation of fun experiments that can be conducted at home extends the reach of this teaching method, providing flexibility for students in various learning environments.

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ZOOM OUT, WAKE UP: CONNECTING CHEMISTRY WITH WHAT MATTERS

Seamus Delaney^{a,*}

^a *School of Education, Deakin University, Australia.*

^{*} *Corresponding author: s.delaney@deakin.edu.au*

Abstract

Students in today's classrooms are aware of global environmental challenges, and they expect their education to provide them the knowledge and skills on how to respond. Given they will live through a period defined by the disruption of climate impacts, they will need to be able to take an active role in supporting both themselves and others to adapt to an ever-changing world. If they don't, society-level decisions will be made for them, likely at a consequence to their economic status and livelihood. This will be the reality for every young person currently in school. Chemistry education must therefore also align to this reality, embedding the knowledge and skills needed for implement a just world across all levels of school curriculum.

Holistic approaches, such as systems thinking, harness contemporary science innovations focused on sustainable development to foster a sense of agency in both teachers and students, empowering them to tackle today's critical societal challenges. However, teaching resources and professional learning opportunities have not kept pace with rapid industry advancements. An ongoing global survey of chemistry schoolteachers¹ is revealing a strong reliance on accessible, curriculum-aligned materials for teaching sustainability. This presentation will showcase recent achievements within the international chemistry education community, offering research-informed strategies to educators who aim to integrate systems thinking into their teaching. It will also remind the audience to not lose sight of the rationale for these curriculum changes: to address societal challenges in all their guises.

Keywords: systems thinking, sustainability, schoolteachers, education

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PET CRADLE-TO-CRADLE RECYCLING

Ruey-Fen (Fanny) Liao*

Executive Vice President of RD, Far Eastern New Century, Taipei, Taiwan

**Corresponding author: fannyliao@feg.com.tw*

Abstract

The central role that industry plays in applying chemistry – the science of transformation of matter – to the production of materials used in every sphere of human activity places the chemical industry to at the forefront of efforts to achieve sustainability for the physical and ecological systems of the planet.¹ Systems thinking helps understand and map the ways that chemistry can contribute to achieving sustainability.²

This panel session in the Symposium on Systems Thinking in Chemistry for Sustainability will provide an overview of challenges and opportunities faced by chemical industry in advancing towards sustainability and the progress being made in the IUPAC Project on Systems Thinking in Chemistry for Sustainability (STCS2030+)³ and the spin-off project Systems Thinking, Sustainability and Chemical Industry (SysTSCI) in which senior members of a number of chemical companies are collaborating.

The speaker will initially present an overview of progress made by the SysTSCI group in developing a case study on sustainable plastics. The panel will further discuss the opening statements with each other and the audience.

PET is the most common recycled plastic around the world. System thinking provides the systematic approach to analyse the PET polymerization from monomers as well as recycling. The presentation would cover the aspects to illustrate “cradle to grave” to “cradle to cradle” recycling of PET through system thinking.

The monomers, PTA and MEG, to produce PET (cradle) could be a petro-based, bio-based and recycled ones. After PET/polyester uses, the post-consumer polymers could be collected for recycling through many different sources such as curb side, recyclable streams, deposit system or ocean collections instead of incineration or landfilled(grave).

The recycling of PET would give the PET a new life (back to cradle). The post-consumer recycling (PCR) of PET/polyester could be conducted via mechanical recycling for single composition plastic containers, physical recycling for single composition polyester fabrics and biological/chemical recycling for complicated PET/polyester mixtures. Each recycling process has its pro and cons in different aspects such as carbon footprint, environmental impacts, cost structure, technology readiness etc.

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3. Systems thinking in chemistry for sustainability: toward 2030 and beyond (STCS 2030+) IUPAC Project No: 2020-014-3

SYSTEMS THINKING, SUSTAINABILITY AND CHEMICAL INDUSTRY: AMMONIA AS AN ENERGY CARRIER

Jeanette Simpson*

Sustainability Manager, Johnson-Matthey, London UK

**Corresponding author: Jeanette.Simpson@matthey.com*

Abstract

The central role that industry plays in applying chemistry – the science of transformation of matter – to the production of materials used in every sphere of human activity places the chemical industry to at the forefront of efforts to achieve sustainability for the physical and ecological systems of the planet.¹ Systems thinking helps understand and map the ways that chemistry can contribute to achieving sustainability.²

This panel session in the Symposium on Systems Thinking in Chemistry for Sustainability will provide an overview of challenges and opportunities faced by chemical industry in advancing towards sustainability and the progress being made in the IUPAC Project on Systems Thinking in Chemistry for Sustainability (STCS2030+)³ and the spin-off project Systems Thinking, Sustainability and Chemical Industry (SysTSCI) in which senior members of a number of chemical companies are collaborating.

The speaker will initially present an overview of progress made by the SysTSCI group in developing a case study on the implications of ammonia as an energy carrier. They will examine the role of ammonia in a hydrogen-based economy to resolve the spatial and temporal differences in availability and demand for renewables⁴. They will also examine how the chemical industry can help address wider system sustainability considerations, such as the planetary boundaries⁵. The panel will further discuss the opening statements with each other and the audience.

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SYSTEMS THINKING, SUSTAINABILITY AND CHEMICAL INDUSTRY: ADVANCING INDUSTRY'S ROLE

Bernard West*

President of Westworks Consulting Limited, Toronto, CANADA

**Corresponding author: bernard.west@sympatico.ca*

Abstract

The central role that industry plays in applying chemistry – the science of transformation of matter – to the production of materials used in every sphere of human activity places the chemical industry to at the forefront of efforts to achieve sustainability for the physical and ecological systems of the planet.¹ Systems thinking helps understand and map the ways that chemistry can contribute to achieving sustainability.²

This panel session in the Symposium on Systems Thinking in Chemistry for Sustainability will provide an overview of challenges and opportunities faced by chemical industry in advancing towards sustainability and the progress being made in the IUPAC Project on Systems Thinking in Chemistry for Sustainability (STCS2030+)³ and the spin-off project Systems Thinking, Sustainability and Chemical Industry (SysTSCI) in which senior members of a number of chemical companies are collaborating.

The speaker will initially present an overview reflecting on previous efforts by industry and highlighting the work of the SysTSCI group in identifying enablers and barriers to industry's transformation towards sustainable production. The panel will further discuss the opening statements with each other and the audience.

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4. Systems thinking in chemistry for sustainability: toward 2030 and beyond (STCS 2030+) IUPAC Project No: 2020-014-3-050

OPPORTUNITIES AND BARRIERS IN THE SUSTAINABLE TRANSFORMATION OF THE CHEMICAL INDUSTRY – A SYSTEMS THINKING APPROACH

Christian Holtze*

*Academic Partnership Developer and Principal Scientist Flow Chemistry,
BASF, Ludwigshafen am Rhein, Germany*

**Corresponding author: christian.holtze@basf.com*

Abstract

Industry plays a central role in applying chemistry – the science of transformation of matter – through the production of materials used in every sphere of human activity. This places the chemical industry at the forefront of efforts to achieve sustainability for the physical and ecological systems of the planet.¹ Systems thinking helps understand and map the ways that chemistry can contribute to achieving sustainability and inform industrial leaders and policy makers, how to efficiently and effectively drive the sustainable transformation of the chemical industry.²

This panel session in the Symposium on Systems Thinking in Chemistry for Sustainability will provide an overview of challenges and opportunities faced by chemical industry in advancing towards sustainability and the progress being made in the IUPAC Project on Systems Thinking in Chemistry for Sustainability (STCS2030+)³ and the spin-off project Systems Thinking, Sustainability and Chemical Industry (SysTSCI) in which senior members of a number of chemical companies are collaborating.

The speaker will initially present an overview of progress made by the SysTSCI group in identifying enablers and barriers to industry's transformation towards sustainable production, aimed at developing a White Paper. Aspects covered will include carbon capture and utilization, renewable feedstock, the role of catalysis and the use of green energy, disposal of chemical products and biodegradation, as well as suggestions to policy makers regarding the emissions trading system, public funding, and the education of students and consumers.

These considerations will be shared in the framework of the opening statements to inspire and provoke a discussion between the members of the panel and the audience.

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4. Systems thinking in chemistry for sustainability: toward 2030 and beyond (STCS 2030+) IUPAC Project No: 2020-014-3-050

SYSTEMS THINKING, SUSTAINABILITY AND CHEMICAL INDUSTRY: SCOPE AND LIMITATIONS OF LIFE-CYCLE ASSESSMENT

Ulla Létinois*

Sustainability Manager Beauty & Care, DSM-Firmenich, Basel, Switzerland

**Corresponding author: ulla.letinois@dsm-firmenich.com*

Abstract

The central role that industry plays in applying chemistry – the science of transformation of matter – to the production of materials used in every sphere of human activity places the chemical industry to at the forefront of efforts to achieve sustainability for the physical and ecological systems of the planet.¹ Systems thinking helps understand and map the ways that chemistry can contribute to achieving sustainability.²

This panel session in the Symposium on Systems Thinking in Chemistry for Sustainability will provide an overview of challenges and opportunities faced by chemical industry in advancing towards sustainability and the progress being made in the IUPAC Project on Systems Thinking in Chemistry for Sustainability (STCS2030+)³ and the spin-off project Systems Thinking, Sustainability and Chemical Industry (SysTSCI) in which senior members of a number of chemical companies are collaborating.

The speaker will initially present an overview of progress made by the SysTSCI group in identifying enablers and barriers to industry's transformation towards sustainable production, with a particular focus on challenges such as gaps in LCA-modeling and -databases and present potential solutions for prospective LCA use as support in e.g. NetZero roadmaps.

The panel will further discuss the opening statements with each other and the audience.

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4. Systems thinking in chemistry for sustainability: toward 2030 and beyond (STCS 2030+) IUPAC Project No: 2020-014-3-050

SYSTEMS THINKING IN THE CHEMISTRY CLASSROOM: TRAINING INSTRUCTORS SO THEY CAN TRAIN THEIR STUDENTS

David A. Laviska^{a,*}, Alisha Szozda^b, Aurelia Visa^c, Felix Ho^d, and Jane Wissinger^e

^aAmerican Chemical Society Green Chemistry Institute;

^bUniversity of Ottawa; ^cCoriolan Dragulescu Institute of Chemistry;

^dUppsala University; ^eUniversity of Minnesota

*Corresponding author: d_laviska@acs.org

Abstract

One of many key differences between curricula for students studying chemistry vs. chemical engineering is that the latter includes systems thinking as a foundational, essential cognitive framework. Chemistry students on the other hand, rarely if ever encounter systems thinking as taught with the intention to inform their understanding of fundamental concepts and skills. There are logical reasons for the divergence of these curricula, but one historical outcome is that chemistry instructors typically lack the expertise to teach through a systems thinking lens (because they themselves were not trained to do so). Therefore, despite the well-proven utility of a systems thinking approach to learning, we have a long way to go toward broad inclusion of this higher-level cognitive approach in the chemistry classroom.

In collaboration with the IUPAC project “Systems Thinking in Chemistry for Sustainability: Toward 2030 and Beyond” (STCS 2030+) we have been assessing perceived barriers for instructors who want to take a systems thinking approach in their chemistry classes so we can develop guidance to support them in overcoming them. At the ACS Green Chemistry Institute, we are working toward a similar goal and have developed several free resources, including a comprehensive learning module for instructors and an asynchronous introductory course that introduces many of the basic systems thinking concepts. In this talk, I will discuss our perception of barriers to systems thinking inclusion with a focus on how they impact instructors. I will also emphasize the urgent need for professional development opportunities that will enable chemistry instructors to more comfortably leverage systems thinking as a powerful teaching tool.

Keywords: Systems Thinking, Instructor Training, Green Chemistry, Sustainability, Professional Development

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SYSTEMS THINKING FOR MATERIAL STEWARDSHIP: IMPLICATIONS FOR CHEMISTRY EDUCATION

Stephen A Matlin^{a*}, Peter G. Mahaffy^c

^a*Visiting Professor, Institute of Global Health Innovation, Imperial College London, UK; and
Vice-President, International Organization for Chemical Sciences in Development*

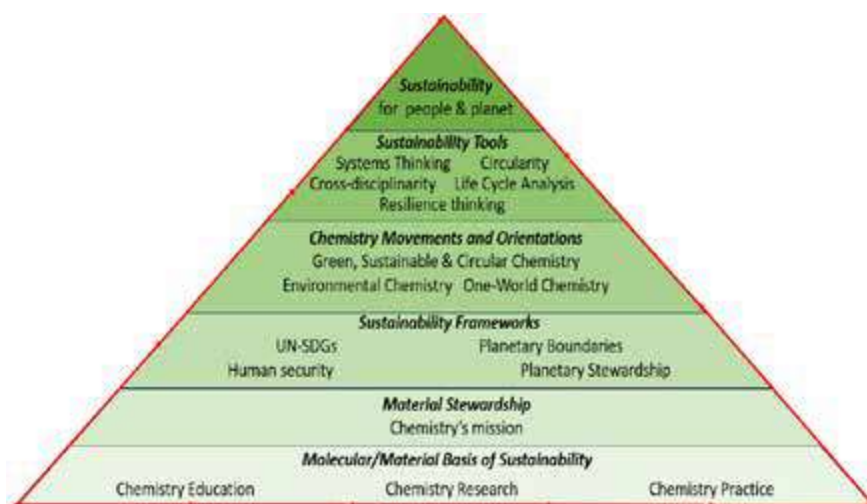
^b*Professor of Chemistry and Director, the King's Centre for Visualization in Science,
The King's University – Edmonton, Canada*

^{*}*Corresponding author: s.matlin@imperial.ac.uk*

Abstract

Adoption of systems thinking helps understand and map the ways that chemistry is involved in the interactions among Earth systems components and how chemistry can contribute to achieving sustainability for the physical and ecological systems of the planet. It is argued that material stewardship should be adopted as a high-priority mission for chemistry.¹ Material stewardship uses systems thinking to take account of all the materials involved in a product – not just focusing on the circularity of the product itself or the security of supply of its raw materials but also factoring in the stewardship of all ingredients, waste products and energy. This approach generates a comprehensive framework within which to situate chemistry's central role as a sustainability science and accords with the understanding that sustainability is an emergent property of the whole system – it is not simply a property of individual elements of the system. Material stewardship interconnects the roles of sustainability frameworks (e.g., Sustainable Development Goals, Planetary Boundaries, Human Security, Planetary Stewardship) and tools (e.g., circular economy, life cycle analysis, systems thinking) with chemistry movements and orientations (e.g., circular, environmental, green, one-world and sustainable chemistry) to achieve sustainability, represented as a 'chemistry for sustainability' pyramid (see Figure below). The mission needs to be adopted by all involved in chemistry education, research and practice. This seminar will explore the scope of material stewardship and the implications for chemistry education of embracing material stewardship as a central mission, presenting some of the concepts and tools that can facilitate teaching and learning, as well as discussing the role of chemical industry.

Keywords: systems thinking, chemistry for sustainability, material stewardship



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SYSTEMS THINKING IN THE LABORATORY CLASSROOM

Thomas A. Logothetis^{a*}

^a *University of Southampton, School of Chemistry and Chemical Engineering,
Highfield, Southampton, SO17 1BJ, United Kingdom*

**Corresponding author: thomas.logothetis@southampton.ac.uk*

Abstract

Systems Thinking^[1] has been well established in most STEM subjects before chemistry picked up on this topic. Meanwhile, Green Chemistry^[2] and Sustainable Development Goals^[3] have been introduced to chemistry curricula in the previous millennium. Yet, they are connected^[4] and this link paves the way to incorporating systems thinking into the chemistry classroom.

The chemistry laboratory is an integral part of chemistry and chemical engineering education. This location and mode of education is precious in many ways (e.g. timewise, financial commitment, infrastructure, teaching workload, health and safety implications) and rightly the trend pushes towards using a laboratory class to focus on dedicated chemistry and transferable practical skills^[5].

With a fragmentation into shorter teaching components, i.e. individual practicals in a laboratory class, it was found inherently more challenging to forge a unit that combines teaching laboratory skills, highlighting progressive sustainable development, and kindling the learners' interest in the bigger picture: systems thinking – the impact of a given “chemistry” on societal, cultural, environmental, economic and other related aspects.

Here, discussion will be examining the challenges encountered by this approach, and how some of these have been overcome, and using this forum to solicit ideas how to best meet remaining issues.

Keywords: Systems Thinking, Laboratory education, Green Chemistry, Sustainability

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EXPLORING RENEWABLE FEEDSTOCKS IN THE CLASSROOM THROUGH SYSTEMS THINKING

Jane E. Wissinger^{a*}

^a*University of Minnesota, Minneapolis, MN, United States*

^{*}*Corresponding author: jwiss@umn.edu*

Abstract

Green Chemistry Principle #7 encourages the use of renewable feedstock “wherever technically and economically practical”.¹ This goal challenges chemists and chemical engineers to invent replacements for the ubiquitous use of depleting fossil fuels that are currently used as the major feedstock for fuels and over 6,000 commercial products. Many academic and industrial researchers are successfully working to make new discoveries using biomass and other renewable materials for applications such as plastics, cosmetics, adhesives, chemicals, lubricants, pharmaceuticals and more, to replace petroleum derived materials. However, a systems thinking analysis of a selected feedstock and application can reveal the complexities of truly meeting the three tenets of sustainability (social, economic, and environmental) by considering the interconnected systems and whether renewable equals sustainable.

This presentation aims to engage students with examples from modern industrial applications of renewable feedstocks (such as corn, soybeans, algae, mycelium, etc..) and those from waste and recycled feedstocks. Chemistry educators should provide the necessary knowledge needed to understand the system under investigation and set appropriate boundaries to guide students in their assignment(s). Case studies can then be used to task students with applying a systems thinking approach to exploring the sustainability aspects of a commercial product considering subsystems such as regional sourcing, energy costs, processing to raw materials, use of water, political ramifications, and more. Application of the SOCKit, SOCME online construction tool provides an interactive and visual representation of the system and subsystems designed. Through these assignments students will build critical thinking skills and an appreciation for the holistic approach needed to solve today’s sustainability challenges defined by the UN Sustainable Development Goals.

Keywords: chemistry curriculum, sustainable chemistry, systems thinking, renewable feedstocks, green chemistry principles,

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RENEWING CHEMISTRY PEDAGOGY: IMPLEMENTING SYSTEMS THINKING IN CHEMISTRY TEACHER EDUCATION

Mageswary Karpudewan

School of Educational Studies, University Sains Malaysia

**Corresponding author: kmageswary@usm.my*

Abstract

A significant trend has emerged in the increasing complexity of global challenges such as climate change, rising energy demands, and newly emerging diseases. These issues are no longer confined to single disciplines; rather, they are multifaceted and span across various fields of study. Therefore, it is essential to prepare students from an early stage in their education to understand and address these complex problems. The reductionist approach to teaching, which is still prevalent in many schools, is insufficient to equip students with the comprehensive knowledge and skills required. Over the past 20 years, my research in green chemistry has demonstrated its effectiveness in providing students with the tools needed to address complex global challenges. While green chemistry has achieved considerable success, integrating systems thinking into green chemistry has further highlighted its interdisciplinary nature.

Systems thinking offers a holistic approach to teaching and learning chemistry, enabling students to participate in discussions, communicate effectively, and make informed decisions about complex issues affecting their local communities (Orgill et al., 2019). Building on this idea, we have integrated systems thinking into green chemistry and introduced it as a renewed pedagogical strategy in the chemistry teaching methods course at Universiti Sains Malaysia. Green chemistry has long served as the foundation of this course, and it has now been enhanced using the framework proposed by Mahaffy et al. (2018).

Initially, student teachers created subsystem concept maps manually. In the most recent semester, we adopted SOCKit—developed by the King's Centre for Visualization in Science, King's University—to assist in creating and exploring these maps. I have been actively involved in training preservice teachers in both systems thinking and green chemistry, recognizing that this is often their first formal experience in learning how to teach chemistry. This initial exposure plays a crucial role in shaping their beliefs and deepening their understanding of new pedagogical approaches. In this presentation, I will share experiences and insights gained from implementing the integrated systems thinking–green chemistry pedagogical strategy.

Keywords: Chemistry, Pedagogy, System Thinking, Teacher Education

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TEXTS IN CHEMISTRY EDUCATION: DIFFICULTIES IN TRANSLATION

Denis M. Zhilin

“Skolca” School, Moscow, Russia

**Corresponding author: zhila2000@mail.ru*

Abstract

Translation of texts in chemistry education is essential for sharing of experience between different nationalities and for chemistry teachers who became displaced persons. However a translator should overcome many difficulties – much more than for chemistry texts.

Any text has three aspects: grammatical (how it is written), semantic (what information it contains) and pragmatic (what is it written for). In grammatical aspect the difficulties depend on the languages; in semantic – on the topic and in pragmatic – on the communities that communicate by translation.

We presume that translated texts are read to apply the described ideas. It is the pragmatic aspect of the translation. If the ideas elaborated within the language L_1 are not applicable for the environment where people speak the language L_2 we get the pragmatic difficulties. Here are the examples.

- “Empty denotate” – the object described by a term from L_1 that is absent in L_2 environment (as the program for training Spartan children “Agoga” for the modern European languages).
- Difference in connotation: a word that has positive connotation in one culture has negative connotation in another.

Semantic aspect gives the wide set of difficulties around the meaning of the terms.

- “False friends”: pedagogical term directly transposed from one language can have completely different meaning in another.
- Ambiguity: a term in one language has several meanings that should be translated by different terms in another meaning.
- Confusions in L_1 : in many texts the terms are used incorrectly and the translation should improve it.
- «Private» systems of terms elaborated by some group of educators claiming that they have invented some new approach whereas they just have renamed or rearranged well-known terms.

To overcome some of these difficulties we launched the project “Multilanguage dictionary of terms in chemistry education”.

Keywords: pedagogical terms, translation, chemistry education

TURKISH TRANSLATION OF MULTI-LANGUAGE DICTIONARY OF TERMS IN CHEMISTRY EDUCATION

Mustafa Sözbilir^{a,*}, Dilek Teke^a

^aAtatürk University, Kazım Karabekir Faculty of Education, Department of Mathematics and Science Education, Chemistry Education, Erzurum-Türkiye

*Corresponding author: sozbilir@atauni.edu.tr

Abstract

Chemistry is a core science with specific terminology. The correct use of terms is important for the correct transfer and understanding of knowledge. A dictionary focusing on terms used in chemistry education research literature is a major deficiency for practitioners and researchers. While there are dictionaries focusing on terms used in chemistry (Somer & Yaşar, 2009) and education (Güneş, 2015), there is no dictionary focusing specifically on terms used in chemistry education literature in Turkish. Therefore, the IUPAC project entitled “Multi-language Dictionary of Terms in Chemistry Education (#2023-031-3-050)” has the potential to fill this gap. The development of this dictionary will be a collaborative effort involving chemistry educators, researchers and experts in the field. The scope of this project includes the production of a dictionary in 16 different languages.

The dictionary has two groups of terms used in chemistry education. The first group of terms are dominated by chemistry content while the second group of terms are coming from pedagogy area. Therefore, it requires a knowledge of both disciplines. This project brought us that there are major problems in this area. Firstly, there is no specific dictionary devoted to chemistry education in Turkish. Secondly, when we translate the terms, we encounter problems finding exact matches. Sometimes, the same English term is translated in different ways in Turkish. This means there is no common term used for anything. On the other hand, there are terms that match with one term in Turkish, while there are several matches in English. Also, there is a limited reference document (e.g. Ayas & Sözbilir, 2017) apart from research papers, in which there is no common language use.

Keywords: Chemistry education, pedagogy, dictionary, translation, Turkish

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WORKSHOP: HOW TO PUBLISH IN CHEMISTRY TEACHER INTERNATIONAL

Mustafa Sözbilir^{a,*}

^a*Atatürk University, Kazım Karabekir Faculty of Education, Department of Mathematics and Science Education, Chemistry Education, Erzurum-Türkiye*
**Corresponding author: sozbilir@atauni.edu.tr*

Abstract

Chemistry Teacher International: Best Practices in Chemistry Education (CTI) is a peer-reviewed open-access journal published by the Committee on Chemistry Education of IUPAC and supported by the Division of Chemical Education of EuChemS. The journal aims to be a platform for teachers of all levels, focusing on researchers in chemistry education. The objectives of the journal are:

- Bridging the gap between research and education
- Creating a platform for all IUPAC activities in the field of education
- Building an international journal not linked to a specific area or nation

The journal is indexed in leading international databases including the Web of Science – Emerging Sources Citation Index Expanded (ESCI, JIF: 2.2) and SCOPUS (CiteScore: 3.1). With these impact factors, CTI is listed among the Q2 journals.

This workshop aims to bring together Editorial Board Members and potential authors face to face to interact. The workshop will cover the following topics:

- Meeting with the Editorial Board Members
- Introduction of aims and scope of CTI, types of manuscripts accepted and policy for the future.
- Basic information about the journal (indexing and citations, statistics for content and coverage etc.)
- Submission and review processes as well as open-access policy and APC payment including APC waive policy of DeGruyter
- Policy of Special issues
- Question & Answers session

Keywords: Chemistry Teacher International, publication papers, journal policy, indexing

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GREEN & SUSTAINABLE CHEMISTRY FOR MAXIMISING AGRICULTURAL PRODUCTIVITY

Antonio F. Patti

Monash University, School of Chemistry, Clayton, Victoria, Australia, 3800

Corresponding author: tony.patti@monash.edu

Abstract

Green and Sustainable Chemistry approaches have a major role in maximising agricultural productivity, while also preserving the environment and protecting human health. The growing need for diverse food sources, more effective fertilisers, pesticides and herbicides with no detrimental human and environmental effects, greener surfactants and greener polymers for agriculture, all require an emphasis on green chemistry approaches.

Agricultural endeavours world-wide are primarily focused on food production. Globally, one third of food produced for human consumption is categorised as lost or waste, which equates to 1.3 billion tonnes per annum. This loss represents the waste of potentially valuable materials such as proteins, simple and complex carbohydrates and lignin (collectively termed lignocellulose), oils and secondary metabolite extractives. In this presentation, several topics and relevant examples for valorising this by-product or discarded biomass will be presented.

A systematic approach first involves determining the chemical composition of the biomass by a variety of standard methods to identify what is valuable¹. Following the identification of the more highly valued and accessible components (eg pectin, pomegranate oil and other extractives) a number of strategies for the extraction and purification of selected components are described².

Other examples of green chemistry applications in agriculture will be covered including: development of an organic based fertiliser for more efficient nitrogen delivery³ and the application of lignocellulose derived hydrogels for water retention in soils⁴.

In all cases, Green and Sustainable Chemistry approaches were applied to give valuable products such as pectin, pomegranate oil and nanocellulose. In addition, a more effective nitrogen fertiliser was achieved as well as the use of by-product lignocellulose for the preparation of a sprayable mulch that could replace current plastic mulches used in the field.

Keywords: Plant biomass, green chemistry, valorisation, pomegranate, fertilisers

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UPCYCLING OF CO₂ AND SPENT POLYESTERS TO VALUABLE CHEMICALS

Yanfei Zhao* and Zhimin Liu*

^a Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, People's Republic of China

*Corresponding author: lianyi302@iccas.ac.cn, liuzm@iccas.ac.cn

Abstract

From the carbon resources viewpoint, CO₂ and spent polymers are important recyclable carbon resources rich on the earth, and their utilization is of great significance to green chemistry and sustainable development. Our research work focuses on the clean and efficient chemical transformation of CO₂ and spent polyesters into useful chemicals. We have designed and synthesized various types of high-performance catalysts (e.g., task-specific ionic liquids and supported nano-catalysts) and developed novel reactions and strategies for their transformation in a green way [1-8]. For example, we have synthesized several CO₂-reactive ILs that can chemically capture and activate CO₂ via forming anion-based carbonate/carbamate intermediates, thus further accomplishing its transformation into quinazoline-2,4(1H,3H)-diones, cyclic carbonates, and benzimidazolones under metal-free conditions [1-4]. We present a hydroxyl carboxylate ILs-catalyzed protocol for depolymerization and transformation of the hydroxyl carboxylic acid-derived polyesters under metal-free and mild conditions, which can accomplish polyester recycling to various chemicals via hydrolysis, alcoholysis, and aminolysis [5]. We developed a ternary catalyst, Ru/CeO₂/RGO, achieving the deconstruction of polycaprolactone into 6-aminocaproic acid and caprolactam, two monomers of nylon-6, using aqueous ammonia without additional H₂ [6]. In addition, we also developed some IL-metal catalyst systems and realized the selective reduction transformation of CO₂ with H₂ [7-8]. For example, we found that Pd/C in 1-butyl-3-methylimidazolium tetrafluoroborate works well for mediating the selectivity of the reaction of cyclic amines with CO₂/H₂, selectively producing N-formamides (at 120 °C) and N-methylamines (at 160 °C) in high yields just by varying the reaction temperature [7]. Moreover, 1,2-bis(N-heterocyclic)ethanes were for the first time obtained from cyclic amines and CO₂/H₂ via McMurry reaction of formamides coupled with subsequent hydrogenation.

Keywords: CO₂ transformation, polyester depolymerization, ionic liquid, nanocatalyst

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TOWARDS GREENER CHEMISTRY: DEVELOPING BENIGN APPROACHES IN ORGANIC SYNTHESIS

Pranjal K. Baruah*

Department of Applied Sciences, Gauhati University, Guwahati-781014, Assam, India.

**Corresponding author: baruah.pranjal@gmail.com*

Abstract

The growing demand for sustainable and environmentally friendly practices has catalyzed a paradigm shift in modern organic synthesis. The development of greener routes to organic molecules not only reduces ecological impact but also enhances the efficiency and practicality of chemical transformations. Among these approaches, metal-free synthesis has emerged as a powerful and transformative strategy, eliminating the use of toxic, expensive, and non-renewable metal catalysts. This aligns seamlessly with the twelve principles of green chemistry, focusing on safety, economy, and sustainability.

Innovative methodologies such as multi-component reactions (MCRs), direct C–H functionalization, and solvent-free protocols have proven invaluable in this pursuit. These techniques enable the construction of structurally diverse and complex organic frameworks with excellent atom economy and minimal waste generation. In particular, the synthesis of heterocyclic compounds — key scaffolds in pharmaceuticals, agrochemicals, and materials science — has greatly benefited from such advancements.

Our research group is actively engaged in developing metal-free, environmentally benign synthetic protocols that are not only cost-effective and scalable but also exhibit high selectivity and efficiency. This presentation will explore recent progress in green synthetic methodologies, with a focus on solvent-free reactions, catalyst-free or organocatalytic approaches, and the design of efficient multi-component systems. These advancements hold the great potential in organic synthesis, offering cleaner, safer, and more sustainable alternatives for future research and industrial applications. Through these efforts, we aim to contribute meaningfully to the global objective of reducing chemical waste and promoting greener chemistry for the benefit of science and society.

Keywords: Green chemistry; metal-free synthesis; multi-component reactions; C-H functionalizations; heterocyclic compounds.

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GREEN OXYGENATION MEDIATED BY GEMINAL-DIOL TYPE SPECIES

Haoran Li*

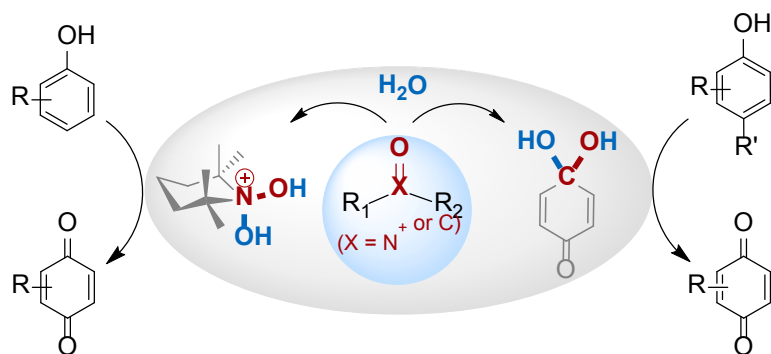
Zhejiang University, Department of Chemistry

*Corresponding author: lihr@zju.edu.cn

Abstract

Oxygenation using water as the oxygen source is a key focus in green chemistry. While geminal diols typically exist in aqueous systems as the hydrated forms of ketones or aldehydes, similar adducts have also been proposed from quinones and oxoammonium cations. Our research has explored the reactivity of geminal-diol type adducts in the oxygenation of phenol compounds, where oxygen is transferred from water to the final products. Using this protocol, we have successfully achieved the oxidation of phenols, the oxidative cleavage of aromatic C–O linkages, and the oxidative cleavage of aromatic C–C bonds, ultimately affording benzoquinone with water as the oxygen source. Moreover, the reduced forms of the oxoammonium cation and quinone—hydroxylamine and hydroquinone, respectively—are easily regenerated through electrochemical methods or aerobic oxidation. This discussion will focus on the oxygenation reactivity of geminal-diol type species and their underlying mechanisms.

Keywords: geminal diol, water, oxoammonium, quinone, oxygenation



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SUSTAINABLE AND PH-RESPONSIVE POLYURETHANE-ACRYLATE FOR ADVANCED DRUG DELIVERY

Choy Sin Lee^{a,*}, Rachel Yie Hang Tan^b, Ki Yan Lam^a and Sit Foon Cheng^c and Mallikarjuna Rao Pichika^d

^aDepartment of Pharmaceutical Chemistry, School of Pharmacy, IMU University, Bukit Jalil, Kuala Lumpur.

^bCentre of Postgraduate Studies, IMU University, Bukit Jalil, Kuala Lumpur.

^cDepartment of Chemistry, Faculty of Science, University Malaya, Kuala Lumpur.

^dNewcastle University, Malaysia.

*Corresponding author: choysin_lee@imu.edu.my

Abstract

pH-Responsive polymers enable controlled drug release by leveraging physiological pH variations. However, conventional polyurethanes rely on non-renewable petrochemical-derived polyols and toxic isocyanates, raising environmental and health concerns. To address this, a sustainable, pH-responsive polyurethane-acrylate (NIPUA) was synthesised via a non-isocyanate route using renewable vegetable oils—palm olein and sunflower oil. The oils underwent *in-situ* epoxidation and a green carbonation reaction under solvent-free conditions to form cyclic carbonate intermediates, which were further reacted with 1,4-butanediamine and bio-based itaconic acid to yield NIPUA. Characterization was performed using FTIR, NMR, and GPC. NIPUA was blended with poly(vinyl pyrrolidone) (PVP) to create a polymer carrier system. Lovastatin (LOV), a hydrophobic model drug, was loaded into the formulations and tested in pH 2.0 and 7.4 media. Differential scanning calorimetry (DSC) confirmed NIPUA's ability to disrupt LOV's crystalline structure, enhancing solubility. Drug release was pH-dependent, with 29.85 µg/mL of LOV released at pH 7.4 versus 22.24 µg/mL at pH 2.0. NIPUA improved LOV solubility by two to four-fold compared to LOV/PVP, pure drug, and marketed tablets (Medostatin). MTT assay results showed increased biocompatibility, with an IC₅₀ of 30.76 µg/mL for pure LOV and 273.53 µg/mL for NIPUA/PVP formulations. This novel, green-synthesized NIPUA, with its pH-responsiveness and solubility-enhancing properties, offers a sustainable alternative to conventional polyurethanes for drug delivery applications.

Keywords: pH-responsive, polyurethane-acrylate, vegetable oil, lovastatin, solubility

SUSTAINABLE SOLUTIONS FOR RECYCLING

Jong-Min Lee¹

*¹Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science and Technology (DGIST),
Daegu 42988, Republic of Korea*

Abstract

The current study focuses on the decontamination and degradation of e-waste plastics. It was estimated that around 25 – 30% of the e-waste consists of plastics. Often the plastics components get destroyed during the metal extraction or disposed of as waste in the landfills and incineration. The e-waste plastics often contaminated with brominated flame retardants (BFRs) and heavy metals such as lead (Pb), chromium (Cr), cadmium (Cd) and mercury (Hg) etc. The presence of toxins makes the e-waste plastics ill-suited for mechanical recycling. In this work novel processes were developed to extract the toxins from e-waste plastics using thermochemical treatments such as extraction and pyrolysis etc. The quantitative analysis of metals and heavy metals present in some of the plastic components of e-waste were found alarmingly higher than the allowable limit. However, BFRs (hexabromocyclododecane (HBCD) and tetrabromobisphenol A (TBBA), etc.) can be precursors to the emission of hazardous polybrominated dibenzo-p-dioxins (PBDD) and polybrominated dibenzofurans (PBDF) under the thermal stress during recycling. Extraction with microwave-assisted extraction (MEA) processes was found efficient in the removal of toxins from the e-waste plastics. Different solvent combination has been tried for optimal result. Different process parameters were optimized for the extraction process.

APPLICATION OF GREEN CHEMISTRY IN INDUSTRIAL POLLUTION CONTRIL

Hossein Ganjidoust*, Bitā Ayati

Tarbiat Modares University, Tehran, Iran.

**Corresponding author: h-ganji@modares.ac.ir*

Abstract

Green Chemistry is a sustainable approach to chemical processes that aims to reduce hazardous materials and pollutants, contributing to a sustainable future. It involves using Fe/C-rich wastes for corrosion inhibitors and creating valuable materials like adsorbents, catalysts, and membranes. Green Chemistry principles address waste management, pollution control, and sustainability, offering environmentally friendly processes, catalytic reactions, and safer organic synthesis. Integrating green chemistry principles into various industries and research fields holds great potential for effective pollution management. The principles of Green Chemistry include waste prevention, atom economy, use of less hazardous chemicals, safer solvents, energy efficiency, renewable raw materials, catalytic methods, degradation-resistant products, analytical methodologies for pollution prevention, and inherently safer processes. These are discussed in this presentation.

Keywords: green chemistry, waste management, hazardous materials, pollution prevention, sustainable environment

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GENERATION OF IN-SITU BLENDED H_2 IN METHANE FROM METHANOL REFORMING

Zohaib Suhail^a, Prince Mishra^a, Alain Goeppert^a, G. K. Surya Prakash^{a,*}

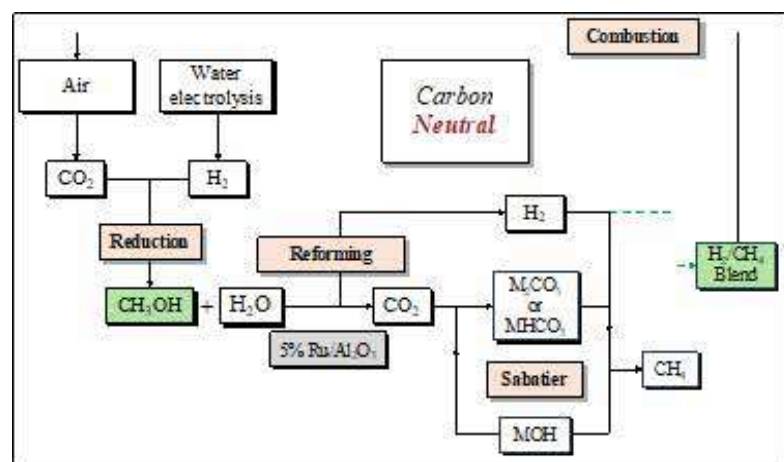
^aLoker Hydrocarbon Research Institute, University of Southern California

*Corresponding author: gprakash@usc.edu

Abstract

Blending hydrogen into natural gas (10-50% H_2/CH_4) has garnered increasing attention as a safe and effective way to reduce carbon emissions.¹ The blend can be directly injected into current infrastructure which eventually accelerates the replacement of fossil fuels, diversifies our energy portfolio, and expedites a net-zero energy future. However, there are intrinsic issues with handling flammable gaseous H_2 such as transport and storage, so a liquid hydrogen carrier would be invaluable. There are also concerns in the carbon footprint of the H_2 and natural gas sources. Methanol, a liquid hydrogen carrier, can be produced by the reduction of captured CO_2 products from flue gas streams or air, rendering it a “green” source. Upon methanol reforming, the CO_2 released can be recaptured to produce more methanol, thus closing the methanol cycle.² Alternatively, CO_2 can also be converted to methane using traditional Sabatier catalysts.³ In this project, we achieved the in-situ generation controllable hydrogen blends ranging from ~10% to 99% via methanol reforming with Ru/Al_2O_3 catalyst and alkali hydroxide salts under batch conditions. We found that methanol first undergoes a disproportionation reaction to form H_2 , formate, and CO_2 . The CO_2 is then captured with a hydroxide to form (bi)carbonates that can be hydrogenated from the internally generated H_2 to methane. The catalyst remained relatively stable throughout multiple reaction cycles. The system is a promising candidate to produce on-site blended hydrogen from green methanol, thus negating the need of mixing gases beforehand.

Keywords: methanol, blended H_2 , dehydrogenation, hydrogen, Sabatier reaction



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HARNESSING BIOLOGICAL INSIGHT: INTEGRATING PROTON REGULATION, pH BUFFER AND ZINCOPHILITY FOR HIGHLY STABLE Zn ANODE

Guolang Zhou, Lili Zhang*

Jiangsu Key Laboratory for the Chemistry of Low-Dimensional Materials, School of Chemistry and Chemical Engineering, Huaiyin Normal University, Huai'an 223001, P. R. China

*Corresponding author: zll@hytc.edu.cn

Abstract

Zinc anodes are severely threatened by hydrogen evolution, dendrite growth and by-products. Inspired by the mechanisms of L-carnosine (L-car) in maintaining intracellular pH stability and fostering mucosal repair in biological systems, this study innovatively proposed a comprehensive strategy integrating proton regulation, pH buffer and zincophilicity by introducing L-car as an electrolyte additive to achieve remarkable stability of zinc anode. Experimental validations and theoretical calculations demonstrate that the abundant N and O sites in L-car can form robust hydrogen bonds with protons, effectively impeding interfacial proton transport and substantially mitigating HER. Moreover, dual pH buffering sites of L-car facilitate dynamic modulation of proton concentration, stabilizing the pH of electrolyte, and suppressing Zn corrosion/passivation/by-product. Concurrently, the robust chelation between L-car and Zn^{2+} orchestrates uniform zinc ion deposition. This synergistic trifecta of L-car endows Zn ion batteries (ZIBs) with an extraordinary cycling stability, extending to an ultralong duration of 5500 hours. Furthermore, the Zn/MnO_2 full battery, demonstrates remarkable stability, retaining a specific capacity of 106.1 mAh/g with 79.2% retention after 1000 cycles at 3 A/g. This study pioneers the interdisciplinary application of L-car in electrolyte modification, presenting a novel paradigm for stabilizing zinc anodes.

Keywords: bio-inspired, Zn anodes, impeded proton transfers, pH buffer, dendrite-free



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MOISTURE RESISTANT K-LOADED ZIF-8 CATALYST FOR GLYCEROL CARBONATE PRODUCTION

Anshu Tyagi^{a, c}, Amjad Ali^{a, c*}, B. N. Chudasama^{b, c}

^aDepartment of Chemistry and biochemistry, Thapar Institute of Engineering & Technology, Patiala 147004, India

^bDepartment of Physics and Material Science, Thapar Institute of Engineering & Technology, Patiala 147004, India

^cAffiliated Faculty – TIET-Virginia Tech, Center of Excellence in emerging Materials, India

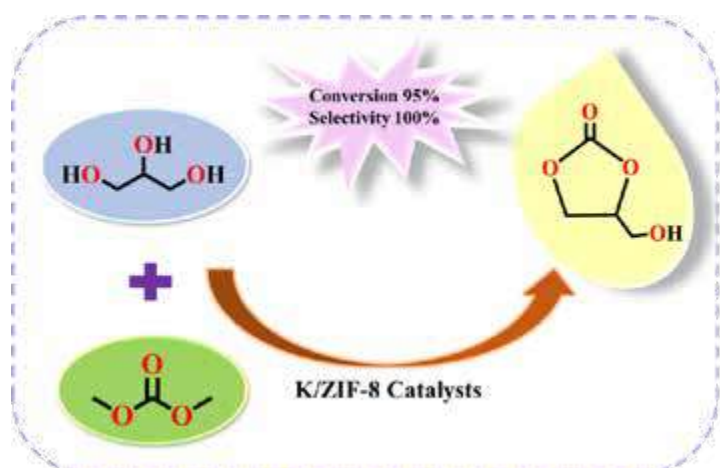
*Corresponding author: amjadali@thapar.edu

Abstract

Zeolitic imidazolate frameworks (ZIFs), a subclass of metal-organic frameworks (MOFs) with structures resembling aluminosilicate zeolites, are gaining significant attention due to their unique properties. ZIF-8, in particular, has shown high surface area and enhanced hydrophobicity, making it a promising candidate for catalytic applications. In this study, ZIF-8 was synthesized in an aqueous medium by mixing 2-methylimidazole (mIm) with zinc nitrate hexahydrate (Zn) in deionized water. To improve the basicity and catalytic performance of ZIF-8, a series of K-loaded ZIF-8 catalysts (K/ZIF-8) were prepared by varying the KOH content from 5 to 10 wt%. Characterization of the synthesized catalysts was conducted using powder X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), high-resolution transmission electron microscopy (HRTEM), and temperature-programmed desorption (TPD) techniques.

The ZIF-8 and K/ZIF-8 catalysts were applied in the transesterification of glycerol (GL) and dimethyl carbonate (DMC) to form glycerol carbonate (GLC). Various reaction parameters, including DMC/GL molar ratio, KOH loading, catalyst amount, and reaction temperature, were systematically studied to optimize the GLC yield. Under optimized conditions, the 10 wt% KOH-loaded ZIF-8 catalyst (10-K/ZIF-8) demonstrated excellent catalytic activity, achieving up to 95% GLC yield at a DMC/GL molar ratio of 3:1 within 0.5 hours. Remarkably, despite the hygroscopic nature of potassium, the catalyst exhibited significant water resistance, maintaining performance with up to 5 wt% water in relation to GL. Furthermore, the catalyst retained its activity after three recycling cycles without any notable loss in catalytic efficiency. This study highlights the potential of K/ZIF-8 as an efficient, water-tolerant catalyst for the transesterification of GL with DMC, offering high GLC yields and recyclability.

Keywords: metal-organic frameworks (MOFs), Zeolitic imidazolate frameworks (ZIFs), transesterification



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DIRECT DISSOLUTION OF LIGNOCELLULOSIC BIOMASS BY MALONIC ACID-DBU FOR HIGH-PERFORMANCE ALL-BIOMASS FILMS

Lifeng Yan*

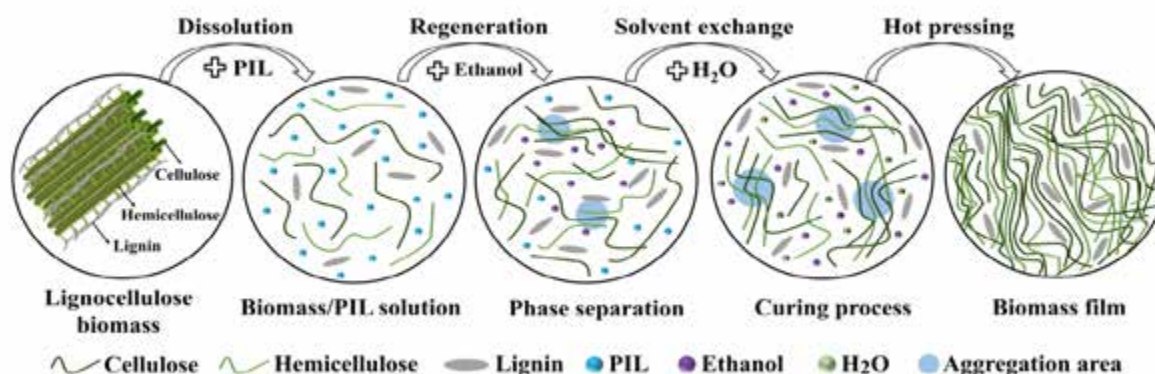
Department of Chemical Physics, University of Science and Technology of China, Hefei, Jinzai Road 96, 230026, Anhui, China..

*Corresponding author: lfyang@ustc.edu.cn

Abstract

Renewable biomass resources have attracted a lot of attention from researchers due to the energy crisis and environmental pollution. The dissolution of biomass is an important topic of biomass refining, so it is crucial to design and develop green solvents. Among them, protonic ionic liquids (PILs) are potential solvents due to the advantages of variety, simple preparation, and low cost. In this work, the direct dissolution of a wide range of biomasses was achieved by using novel malonic acid-DBU PIL. Unlike previous dissolution solvents, this work not only obtained excellent dissolution results (10.2 wt%) but also analyzed in detail the effect of components in the biomass on the dissolution result. The comparative analysis of twelve biomasses summarised the regularity of the components in biomass affecting solubility, which provided instructive information for the field of dissolving biomass by ionic liquids. At the same time, the different types of biomass solutions were practically applied to achieve efficient utilization of resources. The high-performance biomass films with structural integrity, sufficient thermal stability, high tensile strength (107 MPa), excellent UV-blocking (99%), strong water stability, and biodegradability can be prepared by a simple process of coagulation bath regeneration and hot pressing. Moreover, the biomass films retained most of the valuable lignocellulosic fraction, effectively avoiding the waste of biomass resources. In summary, this work achieves the dissolution of biomass by using novel malonic acid-DBU PIL and simultaneously prepares high-performance biomass films, which provide a simple and easy pathway for the conversion and application of biomass

Keywords: lignocellulose, green solvent, dissolving, superbase, ionic liquid, film



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IDENTIFYING ACTIVE SITES WITHIN FULLY EXPOSED CLUSTERS FOR EFFICIENT CYCLOHEXANE DEHYDROGENATION

Mi Peng^a, Ding Ma^{b,*},

^a College of Chemistry and Molecular Engineering, Peking University, Beijing, China

*Corresponding author: dma@pku.edu.cn

Abstract

Understanding the atomic structure of active sites in heterogeneous catalysis is crucial for improving catalytic efficiency. Despite previous research on Pt nanoclusters, the optimal geometry of active sites has remained unclear.¹ This study focuses on the geometric effects of fully exposed platinum (Pt) clusters supported on ceria in cyclohexane dehydrogenation, a reaction pivotal for liquid organic hydrogen carriers (LOHC).

We synthesized Pt clusters with varying sizes on ceria. Comprehensive characterization techniques such as high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM), X-ray absorption spectroscopy (XAS), and density functional theory (DFT) calculations were employed to analyze the structure and performance of the catalysts.

The 0.3Pt/CeO₂ catalyst exhibited superior hydrogen generation activity of 11.4 mol·mol_{Pt}⁻¹·s⁻¹ at 280 °C, outperforming larger Pt particles and single-atom catalysts. Our findings reveal that convex edge sites in fully exposed clusters are primarily responsible for this enhanced activity due to their efficiency in C-H bond activation and resistance to carbonaceous intermediates. The study elucidates a novel structure-performance relationship, demonstrating that these convex edge sites significantly reduce coking and improve catalyst durability. This research provides a new perspective on catalyst design for efficient alkane dehydrogenation processes.

Keywords: cyclohexane dehydrogenation, fully exposed cluster, active sites, hydrogen production

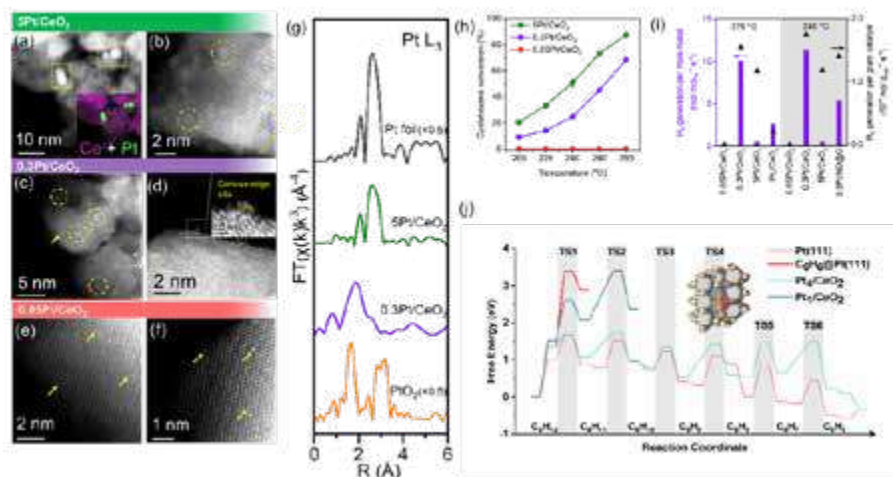


Figure 1. HAADF-STEM of Pt/CeO₂ catalysts (a-f); EXAFS at Pt L₃ edge of Pt/CeO₂ catalysts (g); catalytic performance (h) and comparison with literature (i) for Pt/CeO₂ in cyclohexane dehydrogenation; DFT calculation of cyclohexane dehydrogenation reaction pathway on different Pt/CeO₂ models (j).

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GALACTARIC ACID AS BIO-BASED PLATFORM CHEMICAL

Giacomo Trapasso^{a,*}, Mattia Annatelli^a, Davide Dalla Torre^a, Fabio Aricò^a

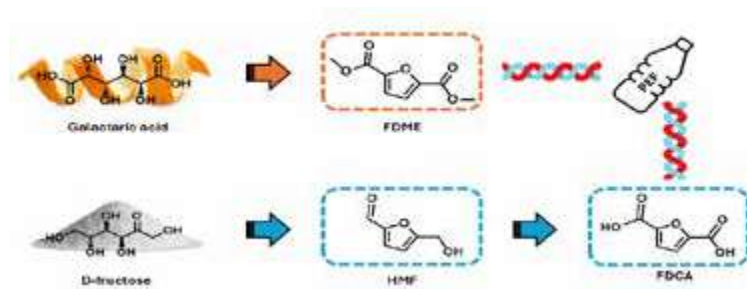
^aDepartment of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice,
Via Torino 155, 30172 Venezia Mestre, Italy.

*Corresponding author: giacomo.trapasso@unive.it

Abstract

2,5-Furandicarboxylic acid (FDCA) has been extensively studied as monomer for the production of polyesters¹ such as polyethylene furanoate (PEF), considered as one of the most valuable bio-based substitute of the petroleum-derived polyethylene terephthalate (PET).² Most of the synthetic processes to FDCA employ glucose and fructose as substrates via the formation of 5-hydroxymethyl furfural (HMF) as key intermediate (Figure 1, top reaction).¹ The main disadvantage of this process regards the intrinsic instability of HMF, together with its high market price and its difficult separation and purification, which ultimately lead to the production of humins, drastically lowering the overall reaction yield. Few studies focused instead on the production of FDCA from alternative substrates. In fact, FDCA can be synthesized starting from aldaric acids, which can be obtained either via oxidation of sugars or directly extracted from citrus peel (Figure 1, bottom reaction).^{3,4} From these premises, the present study reports an alternative synthetic procedure for the production of 2,5-furandicarboxylic acid dimethyl ester (FDME) starting from galactaric acid via dimethyl carbonate (DMC) chemistry. Both sulfonic resins and an iron-based Lewis acid showed to promote the one-pot formation of FDME. The pure product was retrieved as a white crystalline solid with an isolated yield of up to 70 %. Finally, on the basis of the different intermediates identified, a possible reaction mechanism was proposed, which highlights the essential contribute of DMC in the product formation.^{3,4}

Keywords: Bio-based platform chemicals, Galactaric acid, Dimethyl carbonate, Green Synthesis



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CATIONIC POLYELECTROLYTE ENABLES CO₂ ELECTROREDUCTION IN METAL CATION-FREE ACIDIC MEDIA

Jun Gu^{a,*}, Hai-Gang Qin^a

^a*Southern University of Science and Technology, Xueyuan blvd. 1088, Shenzhen, China*

**Corresponding author: guj6@sustech.edu.cn*

Abstract

Room-temperature CO₂ electroreduction is a promising technique to convert renewable intermittent electricity and CO₂ to high-value fuels and chemicals. Recently, CO₂ reduction with acidic electrolyte becomes an emerging hot research topic due to its potential to increase the carbon efficiency.^{1,2} Suppressing the competing hydrogen evolution in the acidic electrolyte is the major challenge. Adding alkaline cations into acidic electrolyte is the most commonly used strategy, which can suppress hydronium reduction by retarding the mass transport of hydronium ions, and promote CO₂ reduction by increasing the electric field strength in electric double layer. However, the addition of alkali cations in the acidic electrolyte leads to bicarbonate precipitation in the gas diffusion electrode, which destroys the hydrophobicity of the electrode and results in flooding. To circumvent the bicarbonate precipitation issue, the most effective strategy is to conduct CO₂ reduction in metal cation free acidic media. In our recent work,³ we covered the electrocatalyst with a cross-linked polyelectrolyte with ultra-high cation density to take over the role of metal cations and achieved highly selective CO₂ reduction in acidic condition free of metal cations. Flooding was substantially suppressed when pure acid solution was used as the electrolyte, and consequently, stable CO₂ reduction Faradaic efficiency was achieved, as demonstrated in the Figure 1. This work provides a strategy to achieve high CO₂ utilization efficiency and good sustainability in CO₂ electroreduction.

Keywords: electrocatalysis; CO₂ reduction; polyelectrolyte; acidic media

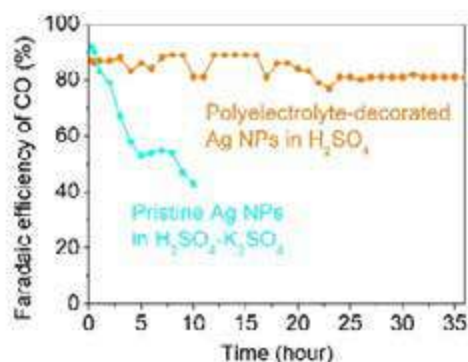


Fig. 1. Comparison of stability of CO₂ reduction in K⁺-containing and K⁺-free acidic electrolyte.

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CHEMICAL RECYCLING OF MIXED TEXTILES: AN UNEXPENSIVE ALTERNATIVE FOR THE SPANDEX ISSUE

Rubio Arias J.J.^{a,*}, Thielemans W^a

^a Sustainable Materials Lab. Chemical Engineering department. Catholic University of Leuven.

Etienne Sabbelaan 53, 8500 - Kortrijk, Belgium

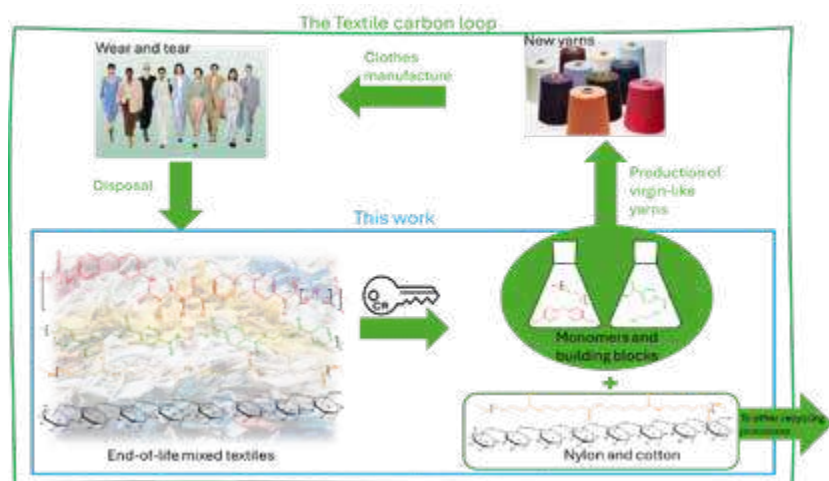
*Corresponding author: josejonathan.rubioarias@kuleuven.be

Abstract

Nowadays, less than 1 % of end-of-life textiles is recycled into new clothes^{1,2} scraps of natural and synthetic polymers in the shape of fibres and yarns are commonly discarded as trash. In order to follow the trends of environmental preservation, we prepared melt-extrusion blends of underwear fabric scraps—made of polyamide-6 and Spandex—and recycled poly(ethylene terephthalate). While mechanical recycling has been applied to some polymers with moderate success (PET bottles), the path for textiles is less clear and normally the end-of-life textiles end up being incinerated, downcycled or sent to landfills. Spandex (or elastane) is a polyurethane:polyurea copolymer made from diamines, diols and diisocyanates³ and voids were observed for samples from untreated fabrics. Thermal analysis indicated that the materials from waste fabrics exhibited both similar melting temperature (around 220 °C). The resulting chemical structure allows for high mechanical resistance and flexibility. Spandex has low thermal stability; therefore, mechanical recycling (re-melting) of spandex-containing textiles becomes unfeasible. In recent years, Chemical Recycling (CR) has gained a lot of attention due to its versatility to address multi-component mixtures, however, when Spandex is present, the CR becomes more challenging and currently there are no feasible solutions for this issue.

The present work demonstrates a new way to deal with Spandex-containing textiles via selective depolymerization of polyesters to reclaim terephthalic acid and glycol, followed by sequential depolymerization of Spandex to reclaim polyols and diamines coming from the Spandex. The method proposed here uses readily accessible chemicals and requires relatively low energy input compared to mechanical recycling. 100% depolymerization of polyester in mixed textiles was achieved in less than 10 min at 50 °C without compromising the structure of spandex. The spandex depolymerization was achieved at 170 °C in less than 1 h to produce diamine and polyTHF, useful building blocks for new polymerizations. The chemical mechanisms, activation energies and influence of additives will be discussed as well as the perspectives and potential for real-life waste streams.

Keywords: Spandex, Chemical recycling, Depolymerization, Textile recycling.



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INORGANIC SALTS CATALYZED CO₂ PROMOTED HYDRATION OF ETHYLENE OXIDE

Dandan Li, Jingshun Zhang, Guohua Gao*

State Key Laboratory of Petroleum Molecular & Process Engineering, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China.

**Corresponding author: ghgao@chem.ecnu.edu.cn*

Abstract

Monoethylene glycol (MEG) has attracted progressively greater attention, as a significant industrial chemical. Recently, we developed a CO₂ promoted hydration of ethylene oxide (EO) for the production of MEG with high efficient and low-cost under low hydration ratio. Herein, we present the strategy of using CO₂ as the reaction atmosphere to promote the hydration of EO catalyzed by simple catalysts of KI/K₂CO₃, with high yields (87.8-98.9%) and selectivities (89.5-99.1%) under hydration ratio of 1.5 (Table 1). Isotope labeling experiments demonstrated that the reaction system proceeds via two distinct pathways. In one pathway, EO undergoes cycloaddition with CO₂ to form ethylene carbonate (EC), which is subsequently hydrolyzed to produce MEG and regenerate CO₂. In the alternative pathway, EO is directly hydrated to produce MEG, in which CO₂ serves as a temporary protective agent to effectively suppress the condensation reaction between EO and MEG (Figure 1). Considering the easy availability of CO₂ and the simplicity and efficiency of KI/K₂CO₃, the current procedure has a potential application in the chemical industry.

Keywords: CO₂, temporary protective agent, KI/K₂CO₃, hydration, ethylene oxide

Entry	Catalysts	Reaction atmosphere	Yield (%)			MEG Select. (%)
			MEG	DEG	EC	
1	KI/K ₂ CO ₃	CO ₂	98.8	0.4	0.4	98.8
2	KI/K ₂ CO ₃	N ₂	56.3	16.9	0.0	62.4
3	None	CO ₂	18.3	9.2	2.3	46.9
4	KI	CO ₂	81.2	0.4	15.3	83.4
5	K ₂ CO ₃	CO ₂	63.3	12.5	-	71.7
6	KBr/K ₂ CO ₃	CO ₂	93.6	1.7	3	93.6
7	KCl/K ₂ CO ₃	CO ₂	75.8	6.9	3.1	81.8
8	KI/Ca ₂ CO ₃	CO ₂	89.6	0.7	5.2	93.1
9	KI/KCl	CO ₂	94.2	0.4	4.9	94.3
10	KI/NaCl	CO ₂	93.7	0.3	1.8	97.5

Reaction conditions: EO (2.2 g, 50 mmol), H₂O (1.35 g, 75 mmol), CO₂/N₂ (0.5 MPa), inorganic salt (2 mol%), inorganic base (1 mol%), 90 °C, 1 h.

Table 1. Hydration of EO catalyzed by inorganic salts under CO₂.

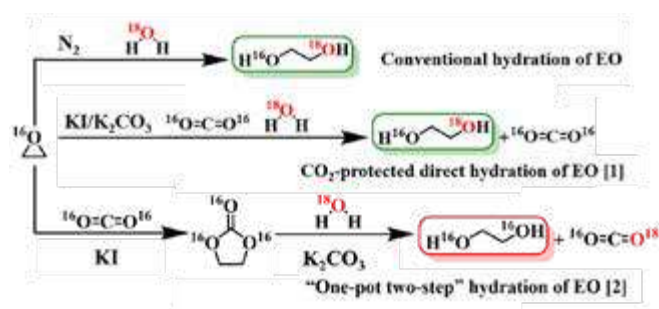


Figure 1. The pathway for hydration of EO under CO₂ or N₂ atmosphere and isotope labeling experiments using isotope-labeled water (H₂¹⁸O).

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PRETREATMENT OF LIGNOCELLULOSE WASTE USING DEEP EUTECTIC SOLVENTS (DESS) FOR BIOFUELS AND CHEMICALS PRODUCTION: STATE-OF-THE-ART, PROSPECTS, AND CHALLENGES

Weidong Lu*

School of Chemistry and Civil Engineering, Shaoguan University

**Corresponding author: louiswdlu@163.com*

Abstract

As the generation of lignocellulose waste escalating, biorefinery of lignocellulose waste for biofuels and high value-added chemicals production has been receiving great concerns from the scientific communities. Renewable, environmentally benign, and biocompatible choline chloride-based deep eutectic solvents (Ch-DESSs) are considered potential alternatives to conventional technologies in the pretreatment of lignocellulose waste. In the past 2 years, numerous innovative studies focused on pretreatment of lignocellulose using Ch-DESSs and process mechanisms have been comprehensively explored. Thus, this review aims to summarize the updated state-of-the-art effort dedicated to pretreatment of lignocellulose using Ch-DESSs. Furthermore, impact factors, kinetic modeling, and chemical mechanisms of the process are thoroughly analyzed and discussed. Finally, prospects and challenges in commercialization of pretreatment of lignocellulose using Ch-DESSs are indicated and extensively discussed.

Keywords: Deep eutectic solvent; lignocellulose waste; biofuels; chemicals

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MICELLE-ENABLED BROMINATION OF α -OXO KETENE DITHIOACETALS: MILD AND SCALABLE APPROACH VIA ENZYMATIC CATALYSIS

Sumrit Wacharasindhu^{a,c*}, Thao Nguyen Thanh Huynh^a, Khuyen Thu Nguyen^a, Chisanu Krongyut^b, Rung-Yi Lai^b, Mongkol Sukwattanasinitt^a,

^aNanotec-CU Center of Excellence on Food and Agriculture, Department of Chemistry, Faculty of Science, Chulalongkorn University Bangkok 10330, Thailand..

^bSchool of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand.

^cGreen Chemistry for Fine Chemical Production and Environmental Remediation Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

*Corresponding author: sumrit.w@chula.ac.th

Abstract

In this study, we demonstrated a bromination of α -oxo ketene dithioacetals using KBr/H₂O₂, catalyzed by the *Curvularia inaequalis* vanadium chloroperoxidase (CiVCPO). A comparative study of enzymatic processes “on water” versus “in water,” using 2% wt of the surfactant TPGS-750-M, revealed that under micellar enzymatic condition, the generation of brominated derivatives of α -oxo ketene dithioacetals was facilitated by enhancing the solubility of starting materials as well as the well dispersion of desired products into the media. This bromination method in an aqueous micellar medium enabled the preparation of brominated α -oxo ketene dithioacetals in fair to excellent yields (23 examples). Subsequently, the gram-scale preparation of brominated α -oxo ketene dithioacetals was performed in the micellar system. The substrate concentration was able to increase up to 50 mM, and the amounts of brominating agents KBr and H₂O₂ were reduced to approximately 2.0 equivalents without compromising efficiency, leading to a more atom-economy process. The key advantages of this method include its benign and eco-friendly nature, the use of water as a green solvent, and which could serve as an alternative for the synthesis of brominated organic compounds. Future research will focus on extending the scope of this reaction to more challenging substrates and further optimizing the system for large-scale production.

Keywords: *Curvularia inaequalis* vanadium chloroperoxidase (CiVCPO), TPGS-750-M, bromination, α -oxo ketene dithioacetals, “on-water” versus “in-water” reactions.

LOW-CARBON CATALYTIC CONVERSION OF BIOMASS AND PLASTICS

Fang Lu*, Xiaoqin Si, Zhiwen Ren, Rui Lu

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China

*Corresponding author: lufang@dicp.ac.cn

Abstract

Under the background of carbon peaking and carbon neutrality, the study on the cleavage of C-C, C-O, and C-H bonds in biomass and plastics is significant for the catalytic conversion of biomass and plastic waste waste to natural gas and hydrogen under mild conditions. Herein, we developed an effective catalytic hydrogenolysis strategy for producing natural gas from various biomass and plastic waste (Figure 1).^{1,2} A catalyst with Ni_2Al_3 alloy phase enables efficient breakage of C-O and C-C bonds in biomass and plastic waste macromolecules under mild conditions, producing natural gas. The total carbon yield of gas products reaches up to 93% after several hours at relatively low temperatures (300 degrees Celsius), which is consistent with the composition of pipeline natural gas. The full life cycle assessment indicated that biomass and plastic -derived natural gas could reduce carbon emissions by about 30% compared with fossil natural gas. Moreover, carbon emissions under normal pressure hydrogen are only about 10% of those under 40 bar hydrogen pressure. The technical economic analysis predicts that the production of biomass and plastic -derived natural gas is economically competitive with a cost price of 380-520 euros/ton. On this basis, low-temperature efficient hydrogen production can be achieved by selective cleavage of C-H bonds in biomass and plastics on the Ni-Mo catalyst.³⁻⁴ Overall, our developed technological routes can effectively reduce carbon emissions with certain economic competitiveness, providing sustainable socio-economic development space for biomass and plastics resources.

Keywords: Biomass; Low carbon; Natural gas; Hydrogen



Figure 1. Scheme on the production of natural gas from biomass and plastics

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SUSTAINABLE UPCYCLING OF SPENT LiCoO_2 BATTERIES AS A HETEROGENEOUS CATALYST FOR BIOMASS VALORIZATION

Emilia Paone^{a,*}, Giulia Maria Itri^a, Francesco Mauriello^a

^a *Dipartimento DICEAM, Università degli Studi Mediterranea di Reggio Calabria, IT89123.*

**Corresponding author: emilia.paone@unirc.it*

Abstract

This study adopts a waste-to-resource approach by repurposing spent lithium cobalt oxide (LiCoO_2 or LCO) batteries, part of a rapidly growing global waste stream, as heterogeneous catalysts for the valorization of lignocellulosic biomass.¹ By utilizing cobalt, a high-value transition metal with exceptional catalytic properties for reductive reactions, this method offers a sustainable alternative to conventional catalysts while mitigating hazardous battery waste.² This approach aligns with circular economy principles by transforming environmental burdens into valuable resources.³

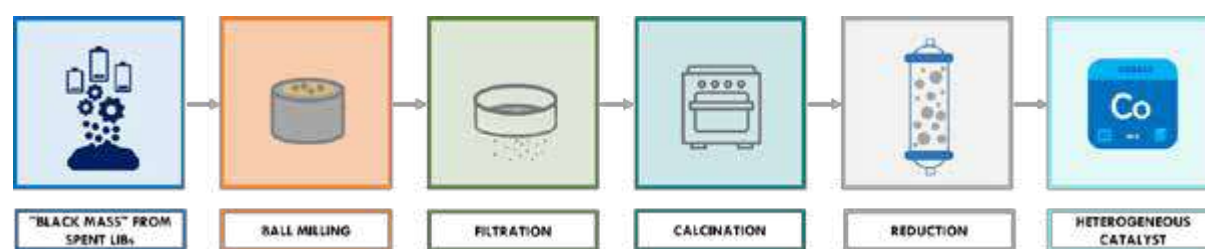
Black Mass (BM), the cathodic material recovered directly from spent LCO batteries, was processed via a simple mechano-thermal treatment to create an efficient cobalt-based catalyst. Detailed characterization of the catalyst was conducted using XRD, FT-ATR, DRIFT, XPS, SEM-EDX, and TEM analyses, confirming its structural and functional properties.

The so-obtained BM catalyst was then tested in the conversion of furfural (FUR) into furfuryl alcohol (FAL), a precious building block widely used in the chemical and pharmaceutical industry, both in the presence as well as in the absence of added hydrogen.

Experiments were performed in a 100 mL stainless-steel autoclave reactor containing 40 mL of a 0.1 M furfural solution and 0.25 g of the BM catalyst.

Under transfer hydrogenation conditions, complete conversion of furfural to furfuryl alcohol was achieved, with a 90% yield after 180 minutes at 180°C. In contrast, classic hydrogenation resulted in lower yields. These findings highlight the BM catalyst's efficiency and potential for sustainable and efficient biomass valorization into high-value chemicals, contributing to renewable energy and resource recovery efforts.

Keywords: Spent Lithium-ion Batteries, Cobalt, Circular economy, Heterogeneous catalysis, Catalytic transfer hydrogenation



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APPLICATION OF RECYCLABLE CARBON NITRIDE PHOTOCATALYST IN VISIBLE-LIGHT MEDIATED SYNTHESIS OF β -KETO SULFONES

Binoyargha Dam^a and Bhisma K. Patel^{b*}

^aThe Assam Royal Global University-Guwahati.

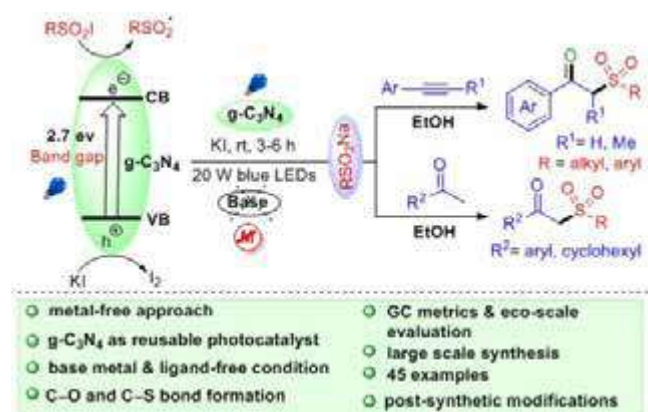
^bIndian Institute of Technology-Guwahati.

*Corresponding author: patel@iitg.ac.in

Abstract

Owing to their easy handling, high stability, and recyclable nature, carbon-based materials have emerged as effective catalytic systems in synthetic organic chemistry.¹ Among others, graphitic carbon nitride (g-C₃N₄) is a metal-free polymer, synthesized by thermal polymerization of easily accessible and cheap starting materials like urea.² Graphitic carbon nitride absorbs light in the visible region (band gap of 2.7 eV; λ_{max} 460 nm) and because of which they have utilized extensively as photocatalyst.¹ Visible-light-mediated reactions are one of the trending topics in modern synthetic chemistry.^{3,4} Herein, this polymeric recyclable heterogeneous photocatalyst was synthesized, characterized and applied for the synthesis of biologically important *b*-keto sulfones in presence of blue light irradiation (Figure 1).⁵ *b*-keto sulfones, were disclosed by using commercially available phenylacetylenes or ketones as precursors and sodium sulfinates, as the sulfonyl source. Potent biologically active compounds like anti-analgesic agents and CES1 inhibitors were synthesized by the present protocol. To explore the applicability, a few post-synthetic modifications of *b*-keto sulfones were also carried out. Finally, to show the greener aspects of the protocol, green chemistry metrics was also calculated. The eco-scale value of the current procedure was also found to be acceptable (with both acetylene and acetophenone). Besides this, metal, base and ligand-free reaction conditions, recyclable photocatalyst (up to five cycles) and wide substrate variability are some additional advantages of this methodology.

Keywords: Visible-light, recyclable photocatalyst, sustainable organic synthesis.



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ELECTROCATALYTIC ACTIVITY OF IRON CENTERS GENERATED WITHIN PHOSPHIDE ENVIRONMENT TOWARD REDUCTION OF NITROGEN TO AMMONIA

Pawel J. Kulesza^{a*}, Iwona A. Rutkowska^a

^a*Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland*

^{*}*Corresponding author: pkulesza@chem.uw.edu.pl*

Abstract

The feasibility of pursuing nitrogen electroreduction reaction, or nitrogen fixation, particularly in aqueous solutions, constitutes an attractive prospect to produce ammonia under ambient conditions. Currently, most of electrochemical approaches to N₂-fixation suffers from slow kinetics due to the difficulty of achieving the appropriate adsorption and activation of dinitrogen leading to cleavage of the strong, triple N≡N bond.

Electrocatalytic systems based on iron phosphides (Fe₂P, Fe₃P) have exhibited electrocatalytic activities toward N₂-reduction reaction in alkaline (NaOH) and semi-neutral (phosphate buffers) media. The results are consistent with the view that, in alkaline medium, the interfacial reduced-iron (Fe⁰) centers within Fe₂P, while existing within the network of P sites, induce activation and reduction of nitrogen, parallel to the water splitting (reduction) to hydrogen. The catalytic system exhibits certain tolerance with respect to the competitive hydrogen evolution; namely, during electrolysis at -0.4 V vs. RHE, the molar efficiency toward production of NH₃ is on the level of 60%. Under such conditions, the NH₃-yield rate has been found to be equal to 7.5 μmol cm⁻² h⁻¹. By referring to classic concepts of electrochemical kinetic analysis, the rate constant in heterogeneous units has been found to be on the moderate level of 1-2*10⁻⁴ cm s⁻¹ (at -0.4 V). Furthermore, by supporting iron phosphides (e.g. Fe₃P) onto hexagonal tungsten nanowires (capable of controlling hydrogen evolution), electroreduction of nitrogen has been feasible in the semi-acid medium (pH=4.6). Finally special attention has been paid to the determination and verification of the identity of the nitrogen-electroreduction products. In this respect, in addition to spectrophotometric and NMR methods, electroanalytical approaches have been explored. A series of diagnostic electrocatalytic experiments have been proposed and performed to control purity of nitrogen gas and to probe presence of potential contaminants such as ammonia, nitrogen oxo-species and oxygen.

Keywords: Nitrogen reduction, iron phosphide catalyst, ammonia, alkaline and semi-neutral media, electroanalytical control experiments

DEVELOPMENT OF HYBRID COPPER-CONTAINING METAL-OXIDE SYSTEMS FOR REDUCTION OF CARBON DIOXIDE IN ACID MEDIUM

Iwona A. Rutkowska^{a*}, Pawel J. Kulesza^a

^a*Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland*

^{*}*Corresponding author: ilinek@chem.uw.edu.pl*

Abstract

There has been growing interest in the electrochemical reduction of carbon dioxide (CO₂), a potent greenhouse gas and a contributor to global climate change, and its conversion into useful carbon-based fuels or chemicals. To produce highly efficient and selective electrocatalysts, the transition-metal-based molecular materials are often considered. To optimize the conventional copper-based electrocatalytic approach, we explore such a model catalytic matrix as nanostructured tungsten oxide nanowires which are capable to undergo partial reduction to hydrogen-rich nonstoichiometric tungsten oxide bronzes. We demonstrate here that following the intercalation of copper into tungsten(VI)-oxide-nanowires, the resulting electrocatalytic systems exhibits synergistic properties toward electroreduction of carbon dioxide. In particular, evidence has been provided that the hybrid Cu/WO₃ catalyst can be successfully utilized to drive reduction of carbon dioxide (saturated solution, concentration, ca. 0.033 mol dm⁻³) in a fairly strong acid medium of 0.5 mol dm⁻³ H₂SO₄. Here formation of the partially reduced tungsten oxides (H_xWO₃ and WO_{3-y}) is accompanied by consumption of protons and sorption of hydrogen, and it tends to inhibit hydrogen evolution by shifting the proton discharge toward more negative potentials. Our observations are consistent with the view that copper is irreversibly trapped (i.e., it cannot be reoxidized) within the network of WO₃ nanowires. On mechanistic grounds, the existence of hydrogen-rich partially-reduced tungsten oxides, H_xWO₃, which contain large population of delocalized electrons and monoatomic H, are likely to induce hydrogenation of carbon oxo species, followed by protonation, in the vicinity of Cu to form oxo-hydrocarbon-type products. Our research aiming at optimization the material's activity and selectivity has also concentrated on application of mixed oxides, e.g. WO₃-ZrO₂. Finally, the present study demonstrates usefulness of certain diagnostic electroanalytical approaches, such as chronocoulometric probing of the diffusional-type charge propagation dynamics, or voltammetric monitoring of small organic or inorganic molecules as electroreduction products.

Keywords: carbon dioxide conversion, electrochemistry, acid medium, hexagonal tungsten (VI) oxide nanowires, hydrogen tungsten oxide bronzes, copper dispersion

VIBRATIONAL SPECTROSCOPY IN PEF-ASSISTED FLAXSEED PROTEIN EXTRACTION: STRUCTURAL CHARACTERIZATION AND RAPID PROTEIN CONTENT PREDICTION

Jervée M. Punzalan^{a,c}, Peter Hartono^{b,c,e}, Sara J. Fraser-Miller^f, Sze Ying Leong^{b,e}, Kevin Sutton^{b,c}, Gert-Jan Moggré^{b,c}, Indrawati Oey^{b,e}, and Keith C. Gordon^{a,b,*}

^a*Dodd-Walls Centre for Photonic and Quantum Technologies and Department of Chemistry, University of Otago, Dunedin 9016, New Zealand*

^b*Riddet Institute, Private Bag 11 222, Palmerston North 4442, New Zealand*

^c*The New Zealand Institute for Plant and Food Research Limited, Private Bag 4704, Christchurch Mail Centre, Christchurch 8140, New Zealand*

^d*Department of Physical Sciences and Mathematics, College of Arts and Sciences, University of the Philippines, Manila, 1000, Philippines*

^e*Department of Food Science, University of Otago, PO BOX 56, Dunedin 9054, New Zealand*

^f*College of Science and Engineering, Flinders University, Adelaide 5042, Australia*

*Corresponding author: keith.gordon@otago.ac.nz

Abstract

Although flaxseed serves as an important source of plant-based proteins, the industry faces challenges in developing efficient, sustainable extraction and analysis methods to satisfy increasing market demands^{1,2}. This study explored pulsed electric field (PEF) technology as a novel extraction enhancement strategy for flaxseed proteins in both aqueous and alkaline conditions, while employing vibrational spectroscopy and chemometric analysis to characterize and quantify protein content in semi-refined flaxseed extracts (SFE). Raman spectroscopy coupled with principal component analysis (PCA) revealed PEF-induced structural modifications in proteins, including changes in secondary and tertiary structures, and disulfide bond conformations. Mid-infrared spectroscopy with second derivative and band deconvolution techniques in the amide I region (1600 cm⁻¹ to 1700 cm⁻¹) estimated secondary structure distribution, revealing that PEF treatment at ~534 kJ/kg in alkaline conditions significantly increased α -helical structures by ~24% while decreasing β -sheet and β -turn content by ~19% and ~13% respectively compared to untreated samples. Near-infrared (NIR) spectroscopy, validated against the Dumas method, demonstrated rapid and accurate protein prediction with root mean square error of prediction (RMSEP) of 0.09% and ratio of performance deviation (RPD) of 8.26 across diverse sample matrices³. Moreover, the study showed that PEF treatment up to 347 kJ/kg enhanced protein content without the need for higher pH or solvents, while higher energy inputs (347-534 kJ/kg) in alkaline conditions increased the extraction of phenolic compounds. This research demonstrates the potential of vibrational spectroscopy and chemometrics for characterizing and monitoring PEF-assisted protein extraction, offering insights into sustainable processing and characterization of complex biomolecular systems.

Keywords: pulsed-electric field, near-infrared, mid-infrared, Raman spectroscopy, chemometrics

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FORMULATION, CHARACTERIZATION AND APPLICATION OF GREEN, EFFICIENT AND LIPASE-BIOCOMPATIBLE BICONTINUOUS MICROEMULSIONS

Xirong Huang^{a,*}

^a Key Laboratory of Colloid and Interface Chemistry of Ministry of Education,
Shandong University, Jinan 250100, People's Republic of China

*Corresponding author: xrhuang@sdu.edu.cn

Abstract

This work focuses on the cutting-edge field of lipase-catalyzed media engineering. To construct a new green and efficient bicontinuous microemulsion medium for the expression of the catalytic activity of surface-active lipase, low vapor pressure hydrophobic ionic liquid with tunable physical / chemical properties and biocompatible zwitterionic amphiphile with low toxicity and good degradability were in this work selected as the oil phase and the surfactant, respectively. Using the fishlike phase diagram method, the microemulsion phase behavior of the pseudoternary system of hydrophobic ionic liquid / water (buffer salt) / zwitterionic surfactant and its evolution with the composition and the structure of hydrophobic ionic liquid and the surfactant were systematically studied, and several zwitterionic surfactant-stabilized hydrophobic ionic liquid-based bicontinuous microemulsions with simple composition, high surfactant efficiency and moderate phase inversion temperature were constructed. The relationship between the phase behavior and the corresponding microstructure of hydrophobic ionic liquid-based microemulsion, which is similar to oil-water system, was confirmed using diffusion nuclear magnetic resonance spectroscopy and other techniques. The component-dependent microemulsion microstructure and the catalytic performance of solubilized lipase were clarified by means of small angle X-ray scattering technology and endogenous fluorescence spectroscopy of lipase. To trace the kinetic process of lipase-catalyzed reaction in a bicontinuous microemulsion system, a chiral high performance liquid chromatography method was developed. The selective hydrolysis of racemic α - phenylethanol ester was chosen as the model reaction, and the medium effect of the bicontinuous microemulsion system on the yield and stereoselectivity of the lipase-catalyzed racemic substrate conversion was illustrated. To recycle lipase in the medium, the temperature-induced phase separation behavior of hydrophobic ionic liquid-based bicontinuous microemulsion was studied, and a green bicontinuous microemulsion medium system for efficient biosynthesis of chiral aromatic alcohols/acids was developed. The above original research not only enriches hydrophobic ionic liquid-based microemulsion systems, but also provides a scientific support for lipase-assisted green biosynthesis of chiral compounds.

Keywords: Hydrophobic ionic liquid, biocompatible zwitterionic amphiphile, bicontinuous microemulsion, lipase, chiral compounds

UPCYCLING DISCARDED COTTON CLOTHING INTO LIGHTWEIGHT MATERIALS USING CELLULOSE NANOFIBRILS

Maria-Ximena Ruiz-Caldas^{a*}, Varvara Apostolopoulou-Kalkavoura^a, Laura Pacoste^a,
Aleksander Jaworski^a, Aji P. Mathew^{a*}

^a Stockholm University – Department of Chemistry

*Corresponding authors: mariaximena.ruizcaldas@su.se aji.mathew@su.se

Abstract

Clothing is an essential part of daily life, but its disposal has a significant environmental impact. One promising way to upcycle cotton textile waste is by extracting cellulose nanomaterials (CNMs), as cotton is the purest source of cellulose among plants.

Cellulose nanofibrils (CNFs) are a type of CNM characterized by a high aspect ratio, flexibility, and their ability to form networks at low concentrations. Currently, they are widely studied for making lightweight materials with high tensile and shear strength, offering an alternative to lightweight materials derived from fossil sources. While alternative cellulose sources like bamboo, hemp, and agricultural residues have been explored for CNF production,^[1] these require extensive purification processes. In contrast, discarded cotton garments, a highly pure source of cellulose, remain underexplored.^[2]

This presentation explores the extraction of CNFs from real discarded cotton textiles. The discarded garments were used “as received” to evaluate the impact of impurities on the final CNF properties. Two functionalization methods were used: cationization using EPTMAC (Cat-Cotton) and carboxylation via TEMPO/NaBr-mediated oxidation (TO-Cotton). These treatments were followed by mechanical fibrillation, resulting in Cat-CNFs and TO-CNFs with distinct morphologies arising from each functionalization route. Both CNF types exhibit high surface charge, small cross-sections, and high aspect ratios.^[3]

The versatility of these textile-based CNFs was demonstrated by fabricating nanopapers and foams. Their properties showed that discarded textiles can be converted into lightweight materials with properties comparable to those derived from virgin sources. This work highlights the potential of using discarded cotton garments as an alternative feedstock for CNF production, offering a new upcycling strategy to convert low-value textile waste into high-value materials.

Keywords: Cotton, textile recycling, nanocellulose, nanofiber, sustainable chemistry



Modified from: Ruiz-Caldas et al., *ChemSusChem* **2024** ^[3]

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SCREENING SINGLE TRANSITION METAL ATOMS ANCHORED ON CARBON NANOTUBES FOR ELECTROCHEMICAL CO₂ REDUCTION

Wuyang Lin^a, Matteo Palma^a and Devis Di Tommaso^{a,b*}

^a Department of Chemistry, School of Physical and Chemical Sciences, Queen Mary University of London, Mile End Road, London, E1 4NS, UK.

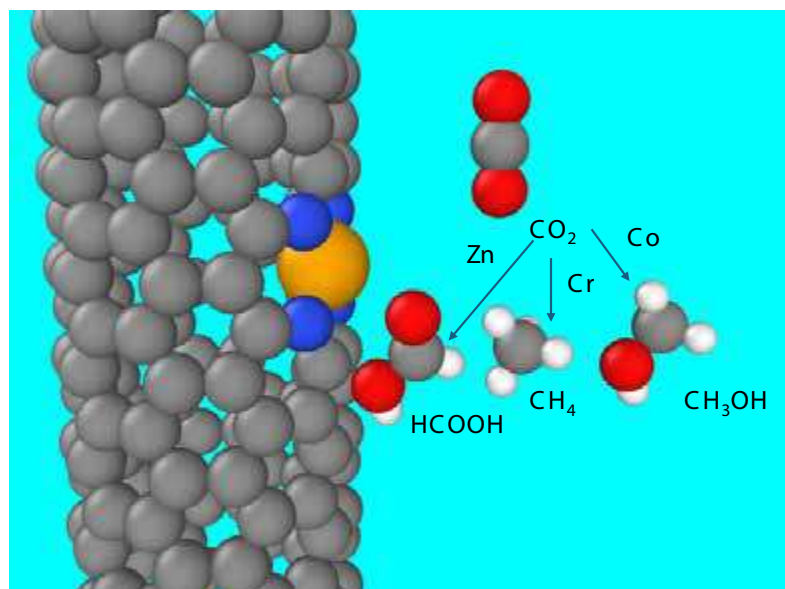
^b Digital Environment Research Institute, Queen Mary University of London, Empire House, London E1 1HH, UK

*Corresponding author: Devis Di Tommaso, d.ditommaso@qmul.ac.uk

Abstract

Single atom catalysts (SACs) are widely used in electrocatalytic reactions due to their superior stability and selectivity. The electrochemical reduction of carbon dioxide (eCO₂R) has garnered significant attention in recent years due to the global warming crisis. However, eCO₂R is still limited by low activity, poor selectivity, and an elusive reduction mechanism. In this work, we investigated the reduction of CO₂ to C1 products catalyzed by nitrogen-coordinated SACs supported on armchair carbon nanotubes (SAC-CNTs). Specifically, we employed a protocol combining density functional theory (DFT) and machine learning simulations to predict the thermodynamic and electrochemical stability, as well as the catalytic performance of SAC-CNTs towards eCO₂R. Our analysis also included the effects of surface curvature and axial strain of the CNTs on catalytic performance. Our results indicate that Cr-N4-CNT and Co-N4-CNT exhibit good selectivity towards CH₄ and CH₃OH, while Zn-N4-CNT is the best candidate for HCOOH formation. Both surface curvature and axial strain influence the relative position of the metal atom on the CNT surface, thereby modulating catalytic activity.

Keywords: electrochemical reduction of carbon dioxide (eCO₂R), single atom catalysts (SACs), density functional theory (DFT), machine learning molecular dynamics (MLMD)



NATURAL REAGENTS AND SMART TECHNOLOGIES FOR GREEN AND SUSTAINABLE CHEMICAL AND PHARMACEUTICAL ANALYSIS: A CASE STUDY ON IRON DETERMINATION

**Kanokwan Kiwfo^{a,b}, Pei Meng Woi^{c,*}, Vannajan Sanghiran Lee^{c,d,*}
Siripat Suteerapataranon^b, Chalermpong Saenjurn^{b,e}, Rujiwatra Apinpus^{b,f}
Kate Grudpan^{a,b,f}**

^aOffice of Research Administration, Chiang Mai University, Chiang Mai 50200, Thailand

^bResearch Center for Innovation in Analytical Science and Technology for Biodiversity-Based Economic and Society (I-ANALY-S-T_B.BES-CMU), Chiang Mai University, Chiang Mai 50200, Thailand.

^cChemistry Department, Faculty of Science, Universiti Malaya, Kuala Lumpur 50603, Malaysia

^dCenter of Excellence in Quantum Information Science and Technology (QiST),
Faculty of Science, Universiti Malaya, Kuala Lumpur 50603, Malaysia

^eDepartment of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University,
Chiang Mai 50200, Thailand

^fDepartment of Chemistry, Faculty of Science, Chiang Mai University,
Chiang Mai 50200, Thailand

*Corresponding author: pmwoi@um.edu.my, vannajan@um.edu.my

Abstract

The shift toward greener and more sustainable analytical methods is transforming chemical and pharmaceutical analysis. This presentation highlights the innovative use of natural reagents, combined with smart technologies such as smartphones and information systems, to drive eco-friendly advancements in chemical analysis. As alternative to synthesized reagents, plant-derived compounds like polyphenols, flavonoids and anthocyanins have been introduced for iron determination in environmental, pharmaceutical, and clinical applications.

Through a detailed case study, we demonstrate how these natural reagents enhance chemical and pharmaceutical analysis with green and sustainability impact. We further present a more advanced evaluation framework integrating green metrics and a refined Need (N), Quality (Q), and Sustainability (S) index. Additionally, we explore the role of blockchain technology in ensuring data transparency, traceability, and sustainability in chemical analysis, setting the stage for a smarter and greener future.

Keywords: Green and Sustainable Analytical Chemistry, Natural Reagents, Smart Technologies, Indexes and Assessments for Greenness and Sustainability, Blockchain Integration

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ELECTROCHEMISTRY AS A POWERFUL TOOL FOR ADVANCING THE FIELDS OF C-H FUNCTIONALIZATION AND HYDROGEN PRODUCTION

Oscar Verho^{*a}

^a*Department of Medicinal Chemistry, Uppsala University, Biomedical Center, Husargatan 3, 751 23 Uppsala.*

Abstract

Electrochemistry has emerged as a versatile tool for enabling redox-driven transformations in organic synthesis and energy conversion. By facilitating controlled electron transfer, electrochemical methods offer a sustainable alternative to traditional chemical oxidants and reductants. In C–H functionalization chemistry, electrochemistry provides a means to activate inert bonds under mild conditions, expanding the scope of direct molecular modifications. Similarly, in water electrolysis, electrochemical approaches drive key bond-breaking and bond-forming steps, enabling the sustainable production of green hydrogen. In the Verho group, we have dedicated considerable research efforts to advance the field of C-H functionalization chemistry and green hydrogen production through the use of electrochemistry as an enabling technology.

In this presentation, several recent C-H functionalization methodologies for carbon-heteroatom bond formation from the Verho group will be highlighted, including (1) a metal-free cascade protocol for the synthesis of halogenated *N*-aryl amides at room temperature,^[1] (2) a cobaltaelectro-catalyzed protocol for the C-H acyloxylation of cycloalkene and arene based 8-aminoquinoline amides at room temperature, and (3) a palladaelectro-catalyzed protocol for the C-H chlorination of heterocyclic scaffolds.^[2] All of these methods demonstrate high chemoselectivity and functional group tolerance, allowing them to be used for the late-stage functionalization of complex molecular scaffolds. Moreover, the presentation will cover the development of novel electrode materials for water electrolysis applications,^[3,4] which open up new exciting opportunities for producing green hydrogen in a more efficient fashion.

Keywords: Electrochemistry, Catalysis, C-H Functionalization, Water Electrolysis, Electrode Design

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SYNTHESIS OF NON-NOBLE METAL CATALYSTS FOR H_2O_2 ELECTROSYNTHESIS

Wenchao Peng*

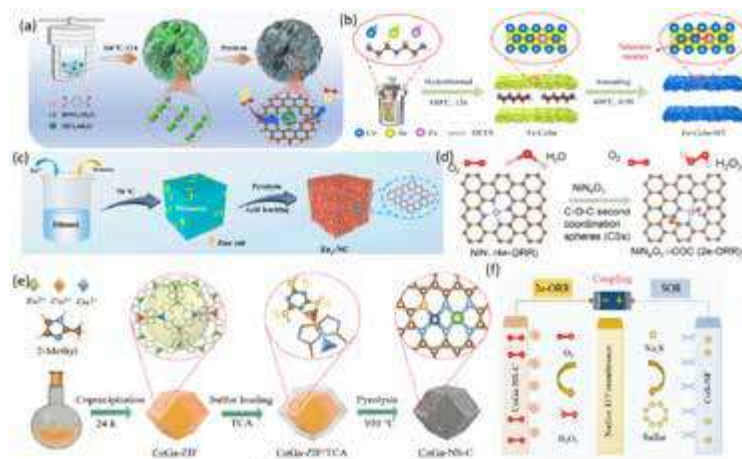
School of Chemical Engineering and Technology, Tianjin University, Tianjin, China.

**Corresponding author: wenchao.peng@tju.edu.cn*

Abstract

Hydrogen peroxide (H_2O_2) is an important chemical, which is widely used in chemical synthesis, medicine, water treatment, and other fields. The production of H_2O_2 via the electrochemical two-electron oxygen reduction reaction (2e^- ORR) is regarded as an alternative route to the anthraquinone method due to its advantages of environmental benignity, high efficiency, and energy saving. Although some noble metal catalysts, such as PtHg and AuPt alloy, exhibit remarkable 2e^- ORR performance, the scarcity limits their actual amplification. While non-noble metals, such as Ni or Co, are always limited by their low activity or selectivity. Here, we have synthesized five different non-noble metal catalysts using hydrothermal or pyrolysis method, which are as follows: (a) NiBi/C alloy catalyst was synthesized by the hydrothermal synthesis of Ni/Bi-MOF and a following pyrolysis process.^[1] (b) The selenium-vacancy-enriched Fe-CoSe-HT catalyst was synthesized through hydrothermal and a further annealing process.^[2] (c) Epoxy group modified atomic Zn- N_2O_2 was synthesized by calcination of a mixture containing melamine and zinc nitrate.^[3] (d) Atomic Ni- N_4O_1 catalyst was screened by DFT calculation and synthesized using a chelation-annealing method.^[4] (e) CoGa-NS-C dual-atom catalyst was synthesized through coprecipitation and S-doped ZIF carbonization treatment with Co and Ga co-doped ZIF-8 as the precursor.^[5] All of the obtained materials exhibit excellent activity for H_2O_2 electrosynthesis via 2e^- -ORR with low overpotential and high yield. The obtained H_2O_2 can be activated by heterogenous CoSe or homogenous Fe^{2+} to degrade kinds of organic pollutants. Moreover, the anodic oxidation of sulfide (f) and 5-hydroxymethyl furfural are used to combine with H_2O_2 electrosynthesis on cathode, thus could decrease the overall voltage for H_2O_2 synthesis and increase its application potential greatly.

Keywords: Hydrogen peroxide, 2e^- -ORR, non-noble metals, single atom, combination



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NEW STRATEGIES FOR MODIFIED ELECTRODE SENSORS USING GREEN DEEP EUTECTIC SOLVENTS AND APPLICATIONS

Christopher M.A. Brett^{a,*}, Joseany M.S. Almeida^a

^a Department of Chemistry, CEMMPRE, ARISE, Faculty of Sciences and Technology,
University of Coimbra, 3004-535 Coimbra, Portugal.

*Corresponding author: cbrett@ci.uc.pt

Abstract

Applications of green Deep Eutectic Solvents (DES), that are based on hydrogen bond interactions, include synthesis, electrodeposition of metals and nanomaterials, as dispersion media for nanoparticles, and preparation of electrochemical sensors, being an alternative to aqueous and non-aqueous solvents, and to ionic liquids [1]. Binary DES are formed by the mixing a single hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD); addition of a second HBD forms a ternary DES (tDES) that can confer improved properties [2]. Some of these systems will be briefly surveyed as well as the green characteristics of DES.

Electroactive redox polymer films on electrode substrates have been prepared by electropolymerization for sensor application [1]. The most common DES for the electropolymerization of phenazine dyes is ethaline (choline chloride and ethylene glycol, molar ratio 1:2) due to its low viscosity, high conductivity, and stability. Such films have been used in electrochemical sensors and biosensors due to their electrocatalytic effect on the oxidation of species such as carboxylic acids and to their favourable electronic, optical, electrochromic, electroluminescent, and chemo-sensitive properties. The combination, in modified electrodes, of electroactive redox polymer films with nanomaterials such as multiwalled carbon nanotubes (MWCNT), graphene (GN), carbon quantum dots (CQD), and metallic nanoparticles has enhanced the sensitivity and electrocatalytic effects of the sensors [3-5]. This has been demonstrated in applications involving analytes such as ascorbate, epinephrine, acetaminophen, 5-aminosalicylic acid, dipyrone, and hydroquinone in pharmaceuticals and dermatological creams. Analysis of samples, such as urine, fruit juices, commercial medications and environmental waters yielded excellent results, indicating that these sensor platforms are promising for future monitoring applications in the environmental, food and clinical contexts.

Keywords: deep eutectic solvents; green solvents; modified electrodes

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UPCYCLING E-WASTE INTO ZINC OXIDE/COPPER OXIDE NANOCOMPOSITES FROM PRINTED CIRCUIT BOARDS FOR PHOTOCATALYTIC WATER TREATMENT

Sheela Chandren^{a,b,*}, Adamu Saidu^a, Nor Arbani Sean^a

^aDepartment of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia

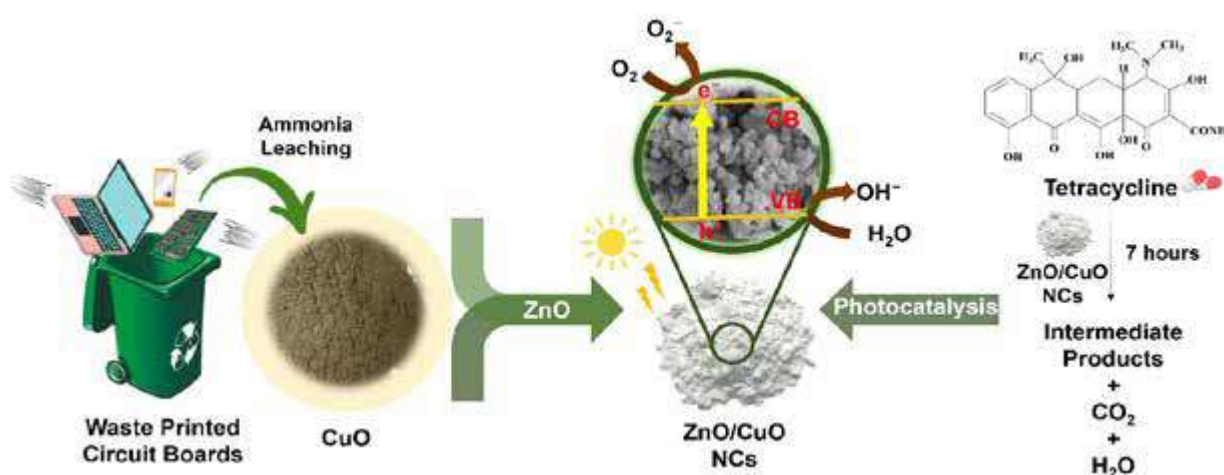
^bCentre for Sustainable Nanomaterials, Ibnu Sina Institute for Scientific and Industrial Research, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia

*Corresponding author: sheela@utm.my

Abstract

The growing consumption of electronic devices has led to environmental concerns, particularly metal contamination and waste accumulation from discarded printed circuit boards (PCBs). However, this challenge presents an opportunity to recover valuable metals and transform them into high-performance nanomaterials. This study utilized the ammonia leaching method to extract copper oxide (CuO) nanoparticles (NPs) from waste PCBs, followed by the synthesis of zinc oxide (ZnO)/CuO NCs at different calcination temperatures (550, 50, and 750 °C) and ZnO precursor concentrations (0.1, 0.2 and 0.3 M). The photocatalytic performance of the NCs was evaluated for tetracycline degradation under visible light irradiation. Results showed that 0.3M-ZnO/CuO-750 NCs achieved the highest degradation efficiency of 73.5% in 7 hours, followed by 0.1M-ZnO/CuO-750 (72.1%) and 0.1M-ZnO/CuO-550 NCs (71.1%). The physicochemical properties of the NCs were extensively investigated using several techniques including Fourier-transform infrared (FTIR), X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), ultraviolet-visible near-infrared (UV-vis-NIR), and nitrogen (N₂) adsorption-desorption analysis. The FTIR spectra proved the existence of the Cu-O bond, Zn-O bond, O-H stretching, and O-H bending that correlate to the functional groups of the NCs. The XRD analysis revealed the distinct peaks corresponding to CuO and ZnO, confirming that ZnO was successfully loaded onto CuO. FESEM revealed particle agglomeration at high calcination temperatures and precursor concentrations. The bandgap energy values varied from 2.22 to 2.74 eV, while the N₂ sorption analysis showed a type IV isotherm with a pore volume distribution of 0.1122 to 0.0278 cm³/g and a surface area of 55.23 to 102.55 m²/g. These findings demonstrate that ZnO/CuO NCs derived from waste PCBs exhibit valuable properties, making them highly promising for sustainable water treatment and electronic waste recycling.

Keywords: printed circuit boards, copper oxide, zinc oxide, tetracycline, photocatalysis



GREEN SYNTHESIS OF ZINC OXIDE NANOPARTICLES USING *CAMELLIA SINENSIS* EXTRACT: AN ECO-FRIENDLY ANTIFUNGAL STRATEGY AGAINST *FUSARIUM EQUISETI* IN NEPALESE TOMATO CULTIVATION

Bimala Subba¹, Ganga Bir Rai¹, Rashmi Bhandari¹, Puja Parajuli¹, Niru Thapa¹,
Dharma Raj Kandel², Sushika Mulmi¹, Sabita Shrestha^{1*} Sailesh Malla³

¹Central Department of Chemistry, Tribhuvan University, Kirtipur, Kathmandu, Nepal

²Department of Bionanotechnology and Bioconvergence Engineering, Jeonbuk National University, 567 Baekje-daero, Deokjin-gu, Jeonju 54896, Republic of Korea

³Strain Improvement Department, Microbe and Culture Research, R&D, Novonesis, Hørsholm, Denmark

*Corresponding author: bimala.subba@cdc.tu.edu.np

Abstract

The emergence of *Fusarium equiseti* as a phytopathogen invading tomato crops in Nepal emphasizes the pressing need for sustainable alternatives to chemical fungicides. A possible environmentally acceptable approach for phytopathogen management is provided by green-synthesized nanoparticles. This study aimed to (1) isolate and identify *F. equiseti* from infected Nepalese tomato crops, (2) biosynthesize zinc oxide nanoparticles (ZnO NPs) using tea leaf (*Camellia sinensis*) extracts via a green chemistry approach, and (3) assess their antifungal efficacy against the pathogen. *F. equiseti* was isolated from infected tomatoes leaves, purified and identified through morphological traits and ITS gene sequencing. ZnO NPs were synthesized using aqueous tea leaf extract under ambient conditions, avoiding toxic reagents. Nanoparticles were characterized via UV-Vis spectroscopy, scanning electron microscopy (SEM), and X-ray diffraction (XRD). Antifungal activity was evaluated in vitro using agar well diffusion method. Our result showed that application of ZnO NPs at 750 ppm to 1200 ppm concentration range inhibited the growth of *F. equiseti* by 77.6% to 85.1% at 7 days of seeding the fungi in PDA media. Microscopic observation of the fungal strain treated with ZnO NPs showed that the presence of the nanoparticles agglomerates the normal hyphae of *F. equiseti* and formed curve tips and breakage of mycelia. This study concluded the successful green synthesis of ZnO NPs with potent antifungal activity against *F. equiseti*. The approach aligns with sustainable agriculture by offering a scalable, nontoxic alternative to synthetic fungicides.

Keywords: Phytopathogen, Fungi, *Fusarium equiseti*, growth inhibition, nanoparticles, tea leaves

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ARTIFICIAL NEURAL NETWORK MODELLING TO OPTIMIZE BIODIESEL YIELD FROM LOW GRADE COOKING OIL USING CALCIUM BASED SUPPORTED ALUMINA

Nursyamimi Zulkurnain¹, Salmiah Jamal Mat Rosid^{2,3*}, Aisyah Fathiah Ahmad¹, Azman Azid¹, Susilawati Toemen⁴, Wan Nazwanie Wan Abdullah⁵, Sarina Mat Rosid¹

¹*Faculty of Bioresources and Food Industry, Universiti Sultan Zainal Abidin, Besut Campus, 22200 Besut, Terengganu, Malaysia*

²*UniSZA Science and Medicine Foundation Centre, Universiti Sultan Zainal Abidin, Gong Badak Campus, 21300 Kuala Nerus, Terengganu, Malaysia*

³*East Coast Environmental Research Institute (ESERI), Universiti Sultan Zainal Abidin, Gong Badak Campus, 21300, Kuala Terengganu, Malaysia*

⁴*Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Skudai, Johor, Malaysia*

⁵*School of Chemical Science, Universiti Sains Malaysia, 11800 Minden, Pulau Pinang, Malaysia*

Corresponding author: salmiahjamal@unisza.edu.my*

Abstract

Biodiesel, is one of the renewable fuels derived from transesterification of vegetable oil such as palm oil, offers a promising alternative. However, the use of homogeneous catalysts in this process presents challenges. These catalysts dissolved in the oil, necessitating large volumes of water for biodiesel purification, which can lead to saponification. In this study, low-grade cooking oil was used as a feedstock for biodiesel production and Ca/Al₂O₃ was used as heterogenous catalyst. The parameters used for the transesterification process included methanol to oil molar ratio (18:1), calcination temperature (400,600,700,800,900 and 1000°C), reaction time (1-3 hours), and catalyst dosage (4-10 wt%) at 60°C of reaction temperature. The optimization was done by using artificial neural network (ANN) design. The potential catalysts were characterized using X-ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-ray (EDX), and Nitrogen Adsorption (NA). The gas chromatography-mass spectrometry (GC-MS) analysis identified palmitic acid as the predominant fatty acid content in the oil. The highest biodiesel yield of 48.30% was achieved under the following conditions: calcination temperature at 800°C, catalyst dosage of 6%, and reaction time of 1 hour. An ANN models demonstrated good agreement with experimental data. The coefficient of determination (R²) value for low-grade cooking oil was 0.9872, indicating superior predictive capability for biodiesel yield. Catalyst characterization by XRD revealed that the Ca/Al₂O₃ catalyst calcined at 800°C had an amorphous structure with BET surface area of 163.4864 m²/g. Meanwhile, FESEM analyses revealed a small particle sizes and irregular shape in the catalysts.

Keywords: biodiesel: low grade cooking oil: artificial neural network: calcium oxide: alumina oxide

ENHANCING PHOTOCATALYTIC ACTIVITY OF REDUCED DENDRITIC FIBROUS TITANIA THROUGH GOLD DEPOSITION

Jaejun Yoo^a and Hyojong Yoo^{a*}

^aDepartment of Battery and Chemical Engineering, Hanyang University ERICA, Ansan, Gyeonggi-do, 15588, Republic of Korea

**Corresponding author: hjhaha73@hanyang.ac.kr*

Abstract

Reduced Dendritic Fibrous Nanotitania (R-DFNT), obtained through the reduction of dendritic fibrous nanotitania precursor (DFNT-Pre), exhibits enhanced photocatalytic activity due to its high light absorption in the UV-Vis region. However, its activity is limited by high electron-hole charge recombination. To tackle this issue, gold nanoparticles were loaded onto the surface of R-DFNT to enhance plasmonic activity. The gold deposition was carried out by directly reducing a gold precursor in an aqueous solution. The plasmonic effect was confirmed by a peak near 550 nm in the UV-Vis spectrum of Au/R-DFNT. The charge-transfer between AuNPs and R-DFNT was observed through the change in binding energy of Au 4f and Ti 2p. The photocatalytic activity of the material was evaluated through the photodegradation of ciprofloxacin (CP). The degradation rate constant of CP by the Au/R-DFNT catalyst was 2.77 times higher compared to that of R-DFNT. Au/R-DFNT has emerged as a potential candidate for utilizing clean solar energy to improve the environment.

Keywords: Gold nano particle, Nanotitania, plasmonic effect, photocatalytic activity

DUAL ANNEALING STRATEGY TO ACTIVATE INERT TUNGSTEN METAL: SYNERGISTIC OPTIMIZATION OF MASS TRANSFER AND ACTIVITY IN CTF-DERIVED ORR CATALYSTS

Huan Ye^a, Yang Li^{a*}

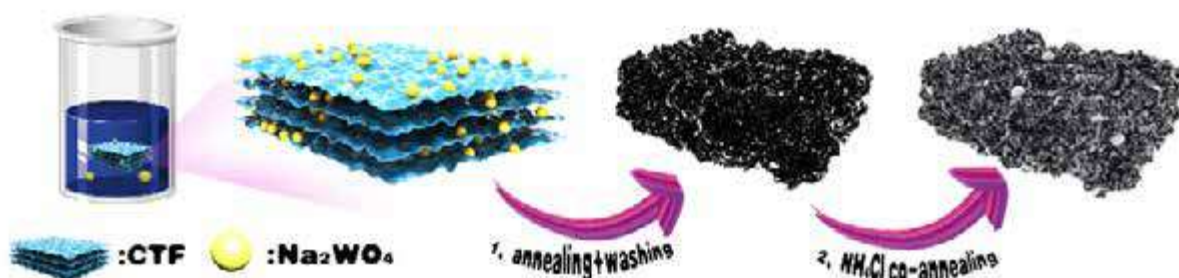
^a*School of Chemical Engineering and Technology, Tianjin University.*

**Corresponding author: liyang1895@tju.edu.cn*

Abstract

Searching for the alternatives to Pt/C catalysts is one of the imperative ways to address the constraints on commercialization of clean energy devices such as fuel cells. Most widely studied non-noble catalysts focus on 3d transition metals such as Fe. However, it has been shown in classical oxygen reduction reaction (ORR) volcano diagram that W exhibits strong oxygen binding energy (ΔE_{O} , similar to Fe), moreover, it shares a similar valence electron structure to Pt. Herein, we designed an alternative W-based ORR catalyst with high catalytic activity via a dual annealing strategy, which solves the critical challenges of mass transfer and catalytic activity in ORR through W precursors serving as self-template and active sites. In-depth analysis via distribution of relaxation time (DRT) and XANES revealed that catalysts with O-doped WN particles active sites exhibited lower mass transfer resistance ($\tau = 0.18$ s) and a higher half-wave potential (0.83 V) compared to W single-atom counterparts (1.6 s, 0.72 V). These values are comparable to Pt/C (0.85 V) in 0.1 M KOH, with superior methanol tolerance. When assembled as a cathode in zinc-air batteries, it achieved a higher open-circuit voltage (1.50 V) and longer stability (140 h) than Pt/C for practical applications.

Keywords: ORR, Mass transfer, catalyst design, clean energy technology



RASPBERRY-LIKE GOLD NANOPARTICLE-DECORATED TITANIA NANORODS FOR PLASMON-ENHANCED PHOTOELECTROCHEMICAL OXYGEN EVOLUTION

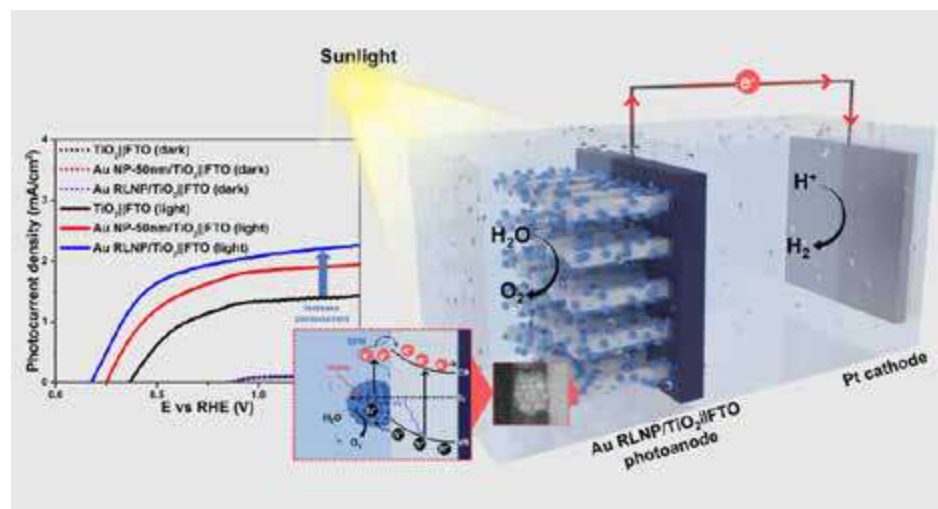
Anisa Fitriani Rosyadi^a and Hyojong Yoo^{a*}

^aDepartment of Battery and Chemical Engineering, Hanyang University ERICA, Ansan, Gyeonggi-do, 15588, Republic of Korea

*Corresponding author: hjhaha73@hanyang.ac.kr

Abstract

The development of efficient photoelectrochemical (PEC) water splitting systems for the oxygen evolution reaction is essential for realizing sustainable hydrogen fuel production. Among the various strategies for enhancing PEC cell performance, plasmonic nanostructures, particularly gold nanoparticles, have emerged as highly promising candidates for improving the efficiency of photoanodes. Herein, we report the fabrication of a photoanode architecture consisting of raspberry-like gold nanoparticles (Au RLNPs) incorporated into hydrothermally synthesized TiO₂ nanorod arrays on a fluorine-doped tin oxide substrate (Au RLNPs/TiO₂//FTO) for photoelectrochemical water splitting application. The Au RLNPs, synthesized via a facile, single-step solution-phase approach, exhibit a distinctive morphology that gives rise to a significantly red-shifted surface plasmon resonance, thereby enhancing visible light harvesting and promoting charge carrier generation. As the result, the Au RLNPs/TiO₂//FTO photoanode demonstrates a remarkable photocurrent density of 2.18 mA·cm⁻² at 1.23 V_{RHE} under AM 1.5G illumination. These findings underscore the substantial potential of the unique photoanode architecture for advancing the development of high-performance PEC water splitting systems.



Keywords: Photoelectrochemical water splitting, gold nanoparticles, raspberry-like morphology, titania nanorods, photoanode, surface plasmon resonance

LAYERED DOUBLE HYDROXIDE-SUPPORTED PALLADIUM NANOCATALYSTS IN SUZUKI-MIYaura COUPLING: A DEPTH REVIEW

Nur Alyaa Kamal^a, Nazrizawati Ahmad Tajuddin^{a,*},

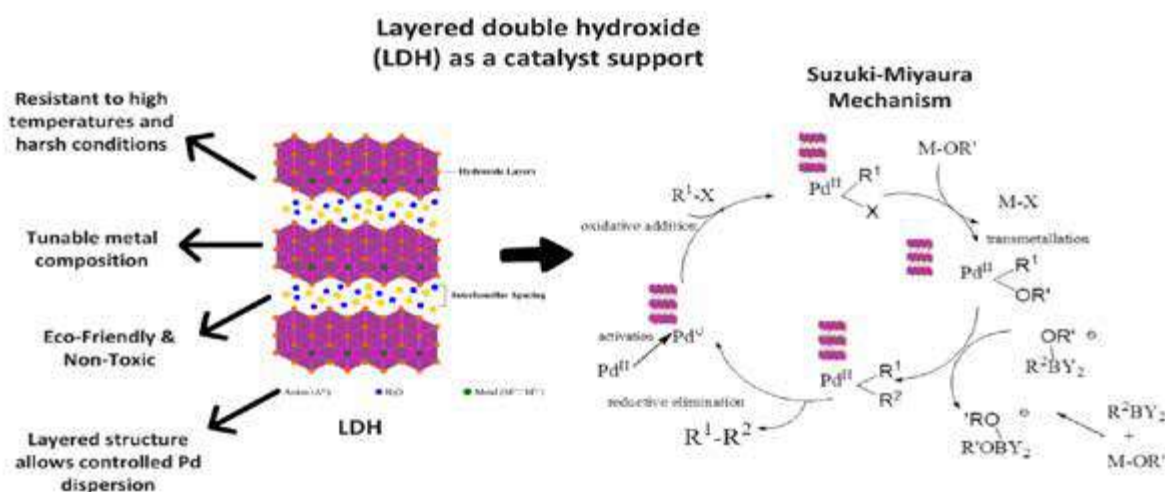
^a*School of Chemistry and Environment, Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia;*

**Corresponding author: nazriza@uitm.edu.my*

Abstract

The Suzuki-Miyaura cross-coupling reaction is a popular method for generating carbon-carbon bonds in organic synthesis, especially in medicines, agrochemicals, and materials research. Palladium-based catalysts are crucial for this reaction, but challenges such as catalyst stability, recyclability, and cost drive the search for improved support materials. In recent years, layered double hydroxides (LDHs) have emerged as promising functional support due to their tunable composition¹, high surface area², and unique basicity², which enhances palladium dispersion and catalytic performance. This review explores the role of LDHs in Suzuki-Miyaura reactions, focusing on their synthesis, structural properties, and influence on reaction efficiency. Additionally, the advantages of LDH-supported palladium catalysts, including improved stability, reduced metal leaching, and recyclability, are discussed as well³. Comparisons of conventional support materials, as well as current challenges and future research directions, are also presented. This review aims to serve as a valuable resource for researchers developing sustainable and efficient catalytic systems for cross-coupling reactions.

Keywords: Suzuki-Miyaura cross-coupling, palladium catalyst, layered double hydroxide, heterogeneous catalysis, sustainable chemistry



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SELECTIVE PRODUCTION OF BIOMASS-DERIVED DIOLS WITH TUNGSTEN-BASED CATALYSTS

Aiqin Wang^{a,*}

^a*Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

^{*}*Corresponding author: aqwang@dicp.ac.cn*

Abstract

Diols are widely used as monomers in polymer industry. Currently, their production mainly relies on fossil resources and involves intensive energy input and CO₂ emissions. From the point of view of sustainability and renewability, the green production of diols from lignocellulose is highly desired yet remains challenging. In this presentation, I will show two examples to demonstrate the catalyst design and process scaling-up for the selective production of low-molecular diols from biomass. The first example is the selective production of ethylene glycol from cellulose. We have developed a variety of tungsten-based binary catalysts for this reaction, and the reaction kinetics and mechanism have been elucidated.¹ The second example is the selective production of 1,3-propanediol from biomass-derived glycerol. For this process, we have developed alumina-supported Pt-W bimetallic catalysts and revealed that the in situ produced Brønsted acid sites by the hydrogen dissociation and spillover to the WO_x are the key active sites for the hydrogenolysis of the secondary C-OH bond of glycerol.^{2,3} Based on the fundamental studies, two pilot demonstrations with a production capacity of 1,000 tons/year have been built for the first time in China, which will pave a way to the development of bio-based polymers.

Keywords: cellulose, biomass-derived diols, tungsten-based catalysts, catalyst design

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STUDY ON THE MULTIFUNCTIONAL APPLICATIONS OF GREEN SYNTHESIZED COBALT OXIDE NANOPARTICLES IN PHOTOCATALYTIC DYE DEGRADATION, ANTIFUNGAL ACTIVITY, AND LPG SENSOR

Nisha Bhattarai, Ganga Bir Rai, Nira Khanal, Bimala Subba and Sabita Shrestha*

Central Department of Chemistry

Tribhuvan University, Kirtipur, Kathmandu, NEPAL

**Corresponding author: sabita.shrestha@cdc.tu.edu.np*

Abstract

Green synthesis of Co_3O_4 NPs using plant products is preferred over that of conventional synthetic procedures because of the economic and environmental benefits. In this research, Co_3O_4 NPs were synthesized by using plant extract of a locally available plant i.e. *Calotropis gigantea*. The phytochemicals like alkaloids, flavonoids, terpenoids, polyphenols etc. present in plant extract can serve as active reducing and capping agents. Here Cobalt (II) acetate was used as a salt precursor with plant extract in nanoparticle synthesis. The synthesized nanoparticles showed two absorption bands around 360 nm and 550 nm. FTIR analysis revealed the strong Co-O bond and various functional groups of metabolic presents in plant extract and XRD analysis demonstrated the size 25.32 nm of the nanoparticles. EDX analysis indicated the presence of cobalt in the biosynthesized nanoparticle. Additionally, synthetic particles were used to test the photocatalytic activity, show that Co_3O_4 NPs can degrade methylene blue (MB) up to 46 % in the presence of sunlight and 9 % in the absence of sunlight. Co_3O_4 exhibits antifungal activity in LL '2' fungi on differing the concentration range and no activity in LL '1' fungi. The films of Cobalt oxide nanoparticles were prepared to test the gas-sensing property in the presence of LPG as test gas.

Keywords: Co_3O_4 NPs, *Calotropis gigantea*, Antifungal activity, Gas sensor, Photocatalytic degradation.

SUSTAINABLE CATALYSIS FOR THE VALORIZATION OF FEEDSTOCK INTO HIGH VALUE CHEMICALS

Shashikant Dighe^{a*}

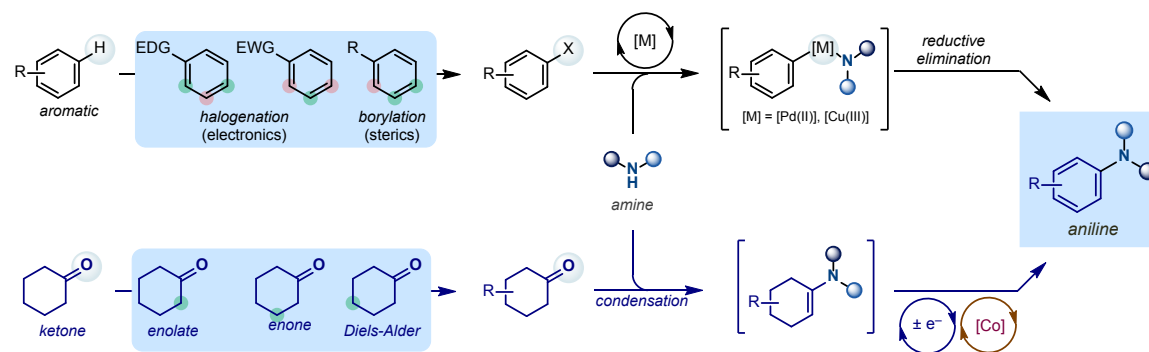
^aAgency for Science, Technology and Research Institute of Sustainability for Chemicals, Singapore

*Corresponding author: Shashikant_dighe@isce2.a-star.edu.sg

Abstract

Nitrogen-containing compounds are a privileged class of molecules, which have applications in medicines, agrochemicals, dyes and materials. This relevance makes the construction of C–N bonds an extremely active area of research. The introduction of amines onto functionalized aromatics at specific and pre-determined positions (ortho vs meta vs para) is currently a prerogative of transition metal-catalyzed processes and requires halogen/boron-containing substrates.¹⁻² The introduction of these groups around the aromatic unit is dictated by the intrinsic reactivity profile of the method (e.g. electrophilic halogenation, C–H borylation) so selective targeting of all possible positions is often not possible. An unconventional cross-coupling strategy for programmable synthesis of anilines on demand, utilizing saturated Cyclohexanones as aryl electrophile surrogates.³ The condensation between amines and carbonyls, a process extensively used by Nature and (bio)organic chemists,⁴ is the enabling feature that ensures a pre-determined and site-selective carbon–nitrogen bond formation, while a synergistic photoredox and cobalt catalytic system is simultaneously employed to progressively desaturate the cyclohexene ring en route to the anilines and N-heterocycles.

Keywords: Cobaloxime, Dehydrogenation, Photoredox catalysis, Feedstock



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HIGHLY POROUS PYROLYZED MIL-101-DERIVED CATALYST FOR THE EFFICIENT DEOXYGENATION OF PFAD INTO GREEN DIESEL

Sivasangar Seenivasagam^{a,b,c,*}, Chang He^{c,d}, Renuga Kannan^{b,c}, Alvin Lim Teik Zheng^{a,b},
 Taufiq Yap Yun Hin^{c,d}

^aInstitute of Ecoscience Borneo, Universiti Putra Malaysia Bintulu Sarawak Campus, Bintulu 97008, Sarawak, Malaysia

^bDepartment of Science and Technology, Faculty of Humanities, Management and Science, Universiti Putra Malaysia Bintulu Sarawak Campus, Bintulu 97008, Sarawak, Malaysia.

^cCatalysis Science and Technology Research Centre (PutraCat), Faculty of Science, Universiti Putra Malaysia, Serdang 43400, Selangor, Malaysia.

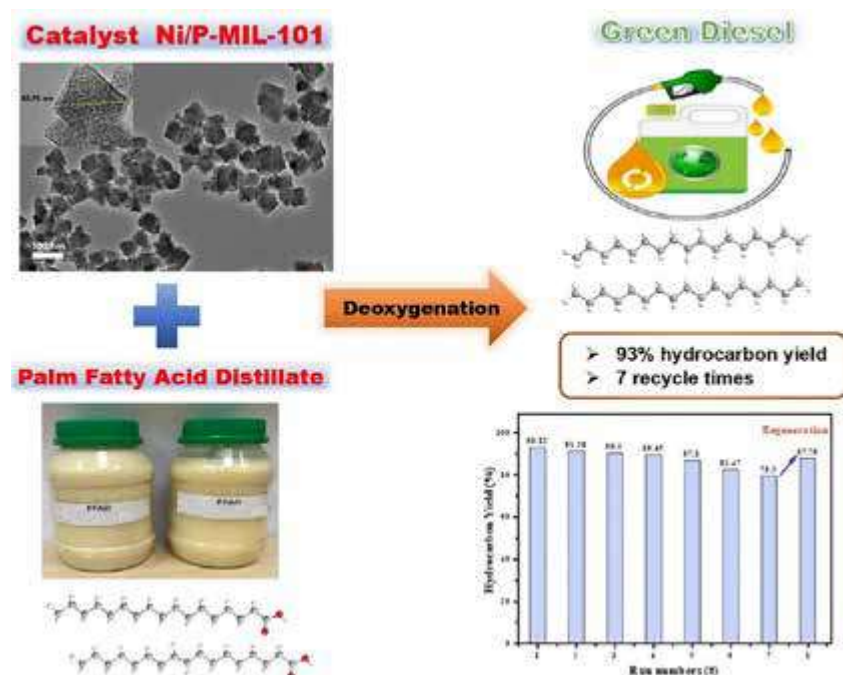
^dDepartment of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

*Corresponding author: sivasangar@upm.edu.my

Abstract

The production of green diesel from renewable, non-edible feedstocks via deoxygenation (DO) presents a sustainable approach to reducing reliance on petroleum-based fuels in the transportation sector. In this study, undiluted palm fatty acid distillate (PFAD) was catalytically converted into paraffinic hydrocarbons using Ni-doped pyrolyzed MIL-101 (MOF-Cr₂O₃) as the catalyst. A series of 4–25 wt% Ni/MOF-Cr₂O₃ catalysts were synthesized through wet impregnation, followed by calcination at 600 °C under an N₂ atmosphere and reduction at 450 °C under H₂ flow. The catalytic DO reactions were conducted at temperatures ranging from 280 to 360 °C with catalyst loadings of 1–7 wt.% and retention times of 1–5 hours under continuous N₂ flow. Among the tested catalysts, 14Ni/MOF-Cr₂O₃ exhibited the highest efficiency, achieving a hydrocarbon yield of 93% with a selectivity of 91% toward n-(C15+C17) at 320 °C within 3 hours using 3 wt% catalyst. The superior performance was attributed to the synergistic effects of well-dispersed Ni species, a high-surface-area support, and the presence of optimized acid-base active sites. Furthermore, preliminary findings indicated that 14Ni/MOF-Cr₂O₃ demonstrated excellent catalytic stability for up to seven cycles, with only a mild reduction in hydrocarbon yield. However, simple regeneration through washing with hexane followed by calcination successfully restored the catalytic activity to a level comparable to the fresh catalyst, highlighting its promising potential for sustainable green diesel production.

Keywords: Biofuel, MOF, Porous Material, Ni Dopant, Renewable Fuel



DEVELOPMENT OF POROUS CE-BASED MOF DERIVED CATALYST FOR SOLVENT FREE LONG CHAIN FATTY ACID CONVERSION TO ELONGATED BIO-WAX KETONE INTERMEDIATES VIA KETONIZATION REACTION

Renuga Kannan^{a,b,c}, Yun Hin Taufiq-Yap^{a,b}, Alvin Lim Teik Zheng^c, He Chang^{a,b},
Sivasangar Seenivasagam^{a, b,c*}

*a. Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400
UPM Serdang, Selangor, Malaysia*

*b. Catalysis Science and Technology Research Centre (PutraCat), Faculty of
Science, Universiti Putra Malaysia, Serdang 43400, Selangor, Malaysia.*

*c. Department of Science and Technology, Universiti Putra Malaysia Kampus
Bintulu, Bintulu 97008, Sarawak, Malaysia.*

**Corresponding author: sivasangar@upm.edu.my*

Abstract

The conversion of palmitic acid (C_{16}) into palmitone (C_{31}) through ketonization presents a promising route for producing bio-based wax compounds. This study focuses on designing a newly developed three-dimensional MnO_2 doped porous carbon catalyst prepared by slowly pyrolyzing a MnO_2 /Ce-MOF precursor at $700^\circ C$ for 4 hours to facilitate this reaction under solvent-free conditions. Characterizations that include XRD, BET, H_2 -TPR, TPD- CO_2 , TPD- NH_3 , TGA, and XPS provided insights into the catalyst's physicochemical properties. Among the varying MnO_2 loading, the 15wt% MnO_2 /P-Ce-MOF composition exhibited the highest catalytic efficiency for palmitic acid ketonization. This is attributed to the formation of balanced acidic and basic sites, which improve feedstock adsorption and promote the ketonization reaction. Under optimized reaction conditions ($340^\circ C$, 3 hours, and 5 wt% catalyst loading), the fresh catalyst achieved a 100% conversion of palmitic acid and a palmitone yield of 86.7%. Upon reuse, the catalyst exhibited excellent reusability, maintaining 100% palmitic acid conversion and a palmitone yield of 71.6% in the second cycle. In subsequent cycles, the catalyst consistently maintained complete palmitic acid conversion (100%), while the palmitone yield gradually decreased. By the fourth cycle, the palmitone yield dropped to 38.2%, with the product composition predominantly consisting of paraffinic hydrocarbons. This research represents a significant advancement in the development of efficient MOF-based catalysts for the solvent-free ketonization of long-chain fatty acids, promoting sustainable approaches for bio-based wax production.

Keywords: Ce-MOF, MnO_2 , Palmitic Acid, Palmitone, Solvent-less

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EXCITED STATE MANAGEMENT AND DEVICE APPLICATIONS OF HIGH MOBILITY EMISSIVE ORGANIC SEMICONDUCTORS

Can Gao^{a,*}, Huanli Dong^{a,*}

^a*Institute of Chemistry, Chinese Academy of Sciences
Zhongguancun North First Street 2, 100190 Beijing, China*

**Corresponding author: cangao@iccas.ac.cn, dhl522@iccas.ac.cn*

Abstract

Organic light-emitting transistors (OLETs) are miniaturized optoelectronic integrated devices that combine the current switching and amplification capabilities of organic field-effect transistors (OFETs) with the electroluminescence functionality of organic light-emitting diodes (OLEDs). OLETs hold significant application potential in emerging display technologies, optical communication, and intelligent sensing. The construction of high-performance OLET devices is essential for their practical applications. A critical approach to achieving high-performance OLETs lies in effectively regulating the excited-state dynamics of the active materials and devices, including exciton migration, recombination, conversion, and annihilation. However, research in this area remains limited, and the underlying photoelectric conversion mechanisms are not yet well understood.

Motivated by these key scientific challenges and building upon our previous work, we have innovatively designed and synthesized a series of high mobility emissive organic semiconductors with superior exciton utilization efficiency and extended exciton transport distances. We have systematically investigated the excited-state behavior and energy loss pathways of these materials in OLETs, providing valuable insights for the development of high-performance, high mobility emissive organic semiconductors. Furthermore, through device structure optimization and fabrication process refinement, we have achieved a significant breakthrough in OLET performance, demonstrating white-light OLETs with an external quantum efficiency (EQE) of up to 13.9%. Additionally, leveraging the unique microcavity effect of OLETs, we successfully developed narrow-spectrum, wide-color-gamut OLETs with a minimum full width at half maximum (FWHM) of 13 nm, advancing their potential applications in relevant fields.

Keywords: organic light-emitting transistor; organic semiconductors; high mobility and strong emission; excited state property; structure-property relationship

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CYCLODEXTRIN ENHANCED ULTRASOUND-ASSISTED EXTRACTION OF BIOACTIVE COMPOUNDS FROM *ZINGIBER MONTANUM*: A GREEN EXTRACTION METHOD

Sirikran Winyupan^a, Catheleeya Mekjaruskul^a, Nadtanet Nunthaboot^b, Vuanghao Lim^c,
Bunleu Sungthong^{a,*}

^aFaculty of Pharmacy, Mahasarakham University, Maha Sarakham, Thailand

^bFaculty of Science, Mahasarakham University, Maha Sarakham, Thailand

^cAdvanced Medical and Dental Institute, Universiti Sains Malaysia, Penang, Malaysia

*Corresponding author: bunleu.s@msu.ac.th

Abstract

A green extraction is considered as an alternative extraction technique concerning reduction of energy consumption or environmentally friendly reagents or chemicals.¹ The use of cyclodextrins (CDs), cyclic oligosaccharides, can improve the extraction yield of bioactive compounds by forming a water soluble inclusion complex between phytochemicals and CDs.² Moreover, a combination of CD with ultrasound-assisted extraction could reduce the extraction time and facilitate the extraction yield by cell wall disruption resulting to the release of phytochemicals. *Zingiber montanum* is a high-demand medicinal plant in Thailand and worldwide due to its biological activities. This study aimed to evaluate the effectiveness of 2-hydroxypropyl β -cyclodextrin (HP β CD) and extraction process on the amounts of bioactive compounds and antioxidant activities from *Z. montanum* rhizome using ultrasound-assisted extraction technique. The extraction model was optimized using response surface methodology by investigating the effects of HP β CD concentration (10 – 30 mM), extraction time (20 – 40 min) and ultrasonic power (140 – 280 W). The responses of the model were the amounts of (*E*)-4-(3',4'-dimethoxyphenyl)but-3-en-1-ol (compound D), (*E*)-1-(3',4'-dimethoxyphenyl)butadiene (DMPBD), curcumin and antioxidant activities. All experiments were performed using water as an extraction medium. The optimization models of all responses exhibited good fits with R^2 more than 0.987. The optimal conditions of each response were ranged 23.78 - 27.65 mM (HP β CD), 30.13 - 31.21 min and 219.16 - 256.75 W. The maxima of all responses were 271.274 μ g/ml (compound D), 525.203 μ g/ml (DMPBD), 20.5634 μ g/ml (curcumin), 494.014 μ M Trolox equivalent (DPPH), 262.412 μ M Trolox equivalent (ABTS) and 510.466 μ M Trolox equivalent (FRAP). Verifications of the predicted and observed values were also performed with relative errors at 0.07 – 4.64%. The optimization of cyclodextrin enhanced ultrasound-assisted extraction of *Z. montanum* rhizome was successfully obtained with high correlation coefficients and low relative errors.

Keywords: antioxidant activity, Inclusion complex, optimization, phytochemicals, response surface methodology

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DEPOLYMERIZING TRANSESTERIFICATION AND AMIDATION OF (POLY) LACTIC ACID ENABLED BY RESONANT ACOUSTIC MIXING

Anton Makarov,^a Magnus Rueping^a

^a*King Abdullah University of Science and Technology*

^{*}*Corresponding author: magnus.rueping@kaust.edu.sa*

Abstract

Increasing production of (poly)lactic acid (PLA) necessitates efficient chemical upcycling methods to reduce waste and capture additional value. This study aims to develop a scalable, green mechanochemical protocol to transform PLA into value-added alkyl lactate esters and lactamides using resonant acoustic mixing (RAM).

Commercial virgin PLA and post-consumer PLA were subjected to organocatalytic depolymerizing transesterification and amidation under RAM conditions. Minimal alcohol or amine equivalents were employed, using no additional solvents or milling media. Catalysis relied on a simple one step-accessible and recyclable guanidine-type base – triazabicyclodecene. The RAM-driven process afforded high yields (up to 90% or more) of alkyl lactate esters and substituted lactamides under mild conditions, eliminating the need for large solvent volumes or bulk grinding media. The method demonstrated excellent scalability, with consistent product yields at gram-to-mole scales within up to 4 hours. The high efficiency of the RAM protocol is believed to stem from the micro-mixing zones generated under RAM conditions, which promote more efficient surface erosion of PLA than conventional stirring.

This RAM-enabled approach offers a sustainable alternative for PLA upcycling by reducing solvent waste and energy input while maintaining high product yields, thereby providing an economically viable pathway toward a circular PLA economy.

Keywords: PLA upcycling, mechanochemistry, resonant acoustic mixing, green chemistry, organocatalysis

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FTIR-CHEMOMETRIC MONITORING OF BIOBASED POLYESTER SYNTHESIS USE FOR PERSONAL CARE APPLICATIONS

Emily S Majanun*, Sara Shahrudin, Irfan Amin Rosli, Wan M Adam Baizuri, Ahmad Zahir Hafiz
Ismail, Nurul Atika Zainuri, Nur Alisya Adriana Nor Azhar, Nurhidayah Rusli

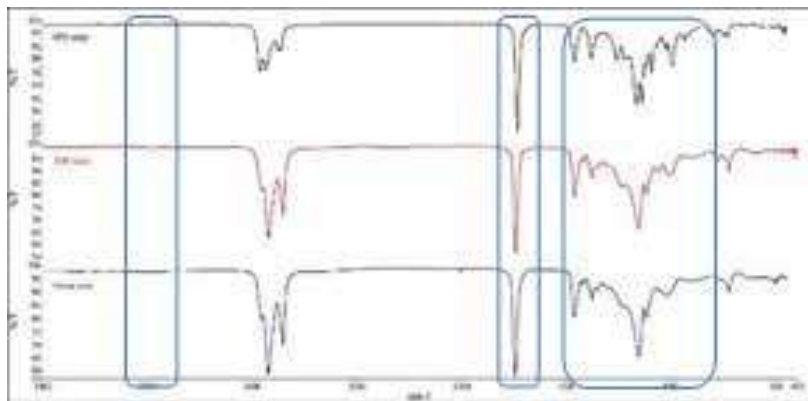
PETRONAS Research Sdn Bhd.

*Corresponding author: emily.majanun@petronas.com

Abstract

This work combines biobased polyesters from multifunctional alcohols—TMP, pentaerythritol, and NPG—reacted with branched fatty acids to produce personal care functional materials. These polyols were selected for their reactivity, structural impact, and skin-contact compatibility. Acid value, hydroxyl value, viscosity, and Fourier-transform infrared (FTIR) spectroscopy were collected at preset intervals to track the esterification reaction in real time, hence providing complete kinetic and structural data. This multiparametric dataset was used to evaluate reaction progress and conversion rates. FTIR data was analyzed using principal component analysis (PCA) and partial least squares regression to obtain insights from evolving chemical fingerprints and overlapping spectral features. By means of superior resolution of complex spectrum data than univariate methods, these chemometric models enhanced response dynamics prediction. For use in emulsions, creams, and lotions, the polyesters have appropriate spreadability and viscosity. Scalable, accurate, and real-time esterification process monitoring is made possible by FTIR-based chemometric analysis coupled with conventional wet chemistry techniques. This approach accelerates the development of personal care products and supports renewable feedstocks and analytical waste reduction in polymer research, thereby increasing sustainability. This work presents a feasible approach to create high-performance, biobased polymers using green chemistry and clean beauty standards.

Keywords: Biobased Polyesters, FTIR Spectroscopy, Chemometric Analysis, Personal Care Polymers



Highlight on the three regions of FTIR used for the fingerprint spectral features.

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SUSTAINABLE CATALYTIC SUPPORTS FROM INSECT-BASED CHITOSAN VIA MECHANOCHEMISTRY

Ana P.C. Ribeiro^{a,*}, Rui P. Oliveira Silva^a, Andreia O. Figueiras^a, Luísa M.D.R.S. Martins^{a,b}

^a Centro de Química Estrutural—Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1, 1049-001 Lisboa, Portugal

^b Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1, 1049-001 Lisboa, Portugal

*Corresponding author: apribeiro@tecnico.ulisboa.pt

Abstract

Mechanochemistry offers an eco-friendly, solvent-free approach to material synthesis, aligning with sustainable development goals. Chitosan, a biopolymer derived from chitin, is gaining attention for its functional properties in catalysis. Recently, black soldier fly (BSF) larvae have emerged as an alternative and sustainable source of chitin, offering a low-cost and circular bioresource. Utilizing chitosan derived from BSF through mechanochemical processes presents a novel strategy for producing catalytic support materials.

This study aims to develop and characterize functional materials from BSF-derived chitosan using mechanochemical methods, targeting their application as supports in heterogeneous catalysis. The goal is to enhance surface reactivity, stability, and catalytic compatibility while promoting valorization of insect biomass.

Chitosan was extracted from BSF larvae through demineralization and deproteinization, followed by deacetylation. The resulting biopolymer underwent high-energy ball milling, both alone and with metal salts (e.g., Cu²⁺, Fe³⁺) to incorporate active sites. Milling parameters were optimized to control particle size, crystallinity, and dispersion of catalytic species. The materials were characterized using FTIR, XRD, SEM, BET, and TGA, and their catalytic performance evaluated in model oxidation and reduction reactions.

Mechanochemical treatment significantly altered the structure of BSF-chitosan, reducing crystallinity and increasing surface area. Effective incorporation and dispersion of metal species were achieved, forming stable bio-based composites. Catalytic tests revealed enhanced activity and good recyclability, confirming the potential of these materials as heterogeneous catalysts. This study demonstrates the viability of mechanochemistry in transforming BSF-derived chitosan into effective catalytic supports. The approach integrates waste valorization with green synthesis, offering a sustainable pathway to advanced functional materials for catalytic applications. The results highlight the potential of insect-sourced biopolymers in circular and green chemistry frameworks.

Keywords: Mechanochemistry, Chitosan, heterogeneous catalysis, Green Chemistry

INTERFACIAL ENGINEERING TOWARD STABLE AH-LEVEL AQUEOUS ZINC BATTERIES

Lina Chen^{a*}, Xuesong Li^a

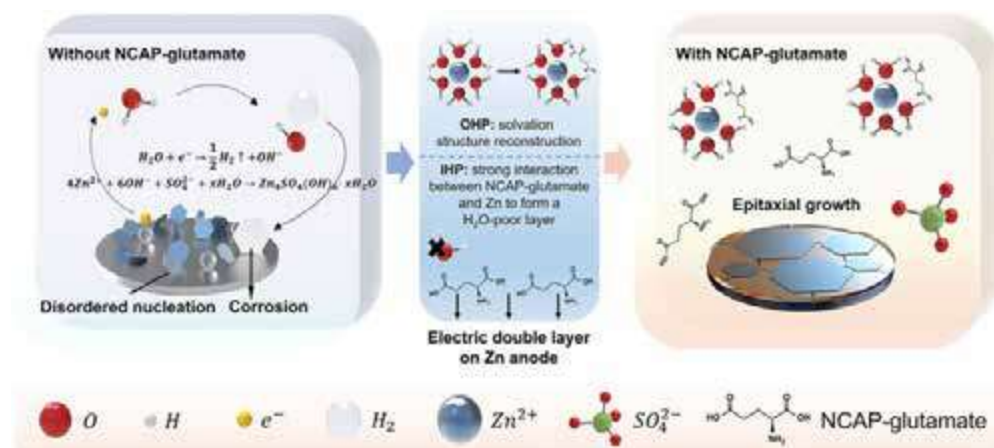
^aShenzhen Institute for Advanced Study, University of Electronic Science and Technology of China, Shenzhen, 518110, China

*Corresponding author: clina92@163.com

Abstract

Aqueous zinc ion batteries (AZIBs) hold great promise as energy storage systems for large-scale applications. However, interfacial instability remains a major challenge, leading to parasitic side reactions and dendrite formation. To address these issues, electrolyte additives-including a bio-derived zincophilic macromolecule and glutamate-were employed to reconstruct the electric double layer (EDL) and regulate zinc deposition behavior. The introduction of these additives leads to the formation of a compact Zn²⁺-rich interfacial layer, uniformly distributed zincophilic sites, and reduced concentration polarization, collectively enabling dendrite-free zinc deposition and highly reversible Zn plating/stripping. As a result, the NH₄V₄O₁₀||Zn full cell achieves a high capacity retention of 82.1% after 3000 cycles at 2 A g⁻¹, and a 1.02 Ah pouch cell demonstrates stable operation over 50 cycles. Furthermore, this work establishes a selection principle to guide the rational design of EDL-reconstructing additives for future electrolyte engineering.

Keywords: aqueous zinc batteries, interfacial engineering, Ah-level



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ALLICIN E - ANTIMICROBIALS - PROVIDING INNOVATIVE SOLUTIONS IN THE FIGHT AGAINST PATHOGENIC MICROORGANISMS

JunWei WANG^{a,*}, JianHua YAO^b, Danny LIN^c,

^a*Chinese Academy of Sciences Shanghai Advanced Research Institute (Chinese Academy of Sciences Innovation Cooperation Center Bangkok).*

^b*Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences.*

^c*Shanghai Landcent Biotechnology*

*Corresponding author: jwwang@casiccb.com

Abstract

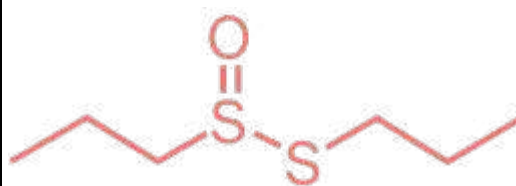
Allicine E is a novel, green, and bioactive small molecule derived from natural garlic extracts and subsequently modified through laboratory techniques to enhance its molecular stability without compromising its potent antimicrobial properties. This breakthrough addresses the long-standing challenge of allixin's instability in its native form, allowing for extended shelf life, broader applicability, and consistent bioactivity under industrial conditions.

The production of Allicine E is designed with sustainability at its core. By utilizing waste streams from fruit and vegetable processing industries, the manufacturing process not only significantly reduces organic waste but also contributes to a circular bioeconomy. This biotechnological approach aligns with global environmental and zero-waste goals, making Allicine E a dual-purpose solution for both public health and sustainable development.

Functionally, Allicine E presents a versatile spectrum of applications. In agriculture and aquaculture, it offers a natural and effective alternative to conventional antibiotics used in animal feed, reducing the risks associated with antimicrobial resistance (AMR). In post-harvest technology, it serves as a biodegradable and non-toxic substitute for parabens in the long-distance transportation and storage of fresh fruits and vegetables, extending shelf life while ensuring consumer safety. Furthermore, Allicine E demonstrates positive effects on soil microbiota when used in agricultural settings, contributing to the restoration of soil health, fertility, and long-term productivity.

In conclusion, Allicine E represents a next-generation antimicrobial agent that combines natural efficacy, enhanced stability, industrial scalability, and strong sustainability credentials. Its multifunctional benefits position it as a transformative solution for health-conscious, eco-responsible, and innovation-driven food and agricultural systems worldwide.

Keywords: Green, Agriculture, Antimicrobiol, Materials, Farming



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THE ION BEHAVIOR AND STORAGE MECHANISM OF 2D MoO_3 LAYER STRUCTURE IN AN AIR-STABLE HYDRATED EUTECTIC ELECTROLYTE FOR ALUMINUM-ION ENERGY STORAGE

Feng Hao Hsu^a, Su Yang Hsu^b, Ramesh Subramani^b, Tsung Chia Cheng^b, Bo Hao Chen^b, Jeng Lung Chen^b, Kueih Tzu Lu^b, Jin Ming Chen^c

^aDepartment of Applied Chemistry, Providence University, Taichung, 43301, Taiwan

^bNational Synchrotron Radiation Research Center, Hsinchu, 30076, Taiwan

^cDepartment of Electrophysics, National Yang Ming Chiao Tung University (NYCU), Hsinchu 30010, Taiwan

*Corresponding author: jmchen@nycu.edu.tw

Abstract

The α - MoO_3 material with a two-dimensional (2D) layer structure is proposed as a promising cathode material for aluminum-ion (Al-ion) energy storage in the air-stable $\text{Al}(\text{ClO}_4)_3 \cdot 9\text{H}_2\text{O}$ /succinonitrile hydrated eutectic electrolyte (ASHEE) system. The electrochemical measurements reveal that the α - MoO_3 electrode material exhibits a high capacity of approximately 285 mA h g^{-1} , a wide potential window of 2 V, and the capacity retention of approximately 86 % after 40 charge/discharge cycles at a current density of 0.4 A g^{-1} . The correlation between electrochemical performance and crystal structure of α - MoO_3 electrode material is investigated using *in-situ* X-ray absorption spectroscopy (XAS) and X-ray diffraction (XRD) techniques. The results highlight the favorable attributes of α - MoO_3 as a cathode material in the ASHEE system for Al-ion energy storage, including high safety, air-stability, exceptional electrochemical performance, and low cost. This study provides detailed insight into the electrochemical performance and ion storage mechanism of the 2D α - MoO_3 cathode material, paving the way for its application in future promising electrolyte systems for Al-ion energy storage. The findings contribute to the advancement of Al-ion energy storage technology by offering a comprehensive understanding of the electrochemical performance and storage mechanism of 2D α - MoO_3 as a cathode material in the ASHEE system, facilitating the development of efficient, safe, and cost-effective Aluminum-ion battery.

Keywords: molybdenum trioxide, air-stable electrolyte, *in-situ* XAS, *in-situ* XRD, Al-ion energy storage

GREENER AND RAPID MAGNETIC SOLID PHASE MICROEXTRACTION METHOD USING $\text{Fe}_3\text{O}_4@\text{Al}_2\text{O}_3/\text{AC}$ FOR CHROMATOGRAPHIC DETERMINATION OF NEONICOTINOID PESTICIDES IN VEGETABLE OILS

Musiwa V. Sengane^a, Masixole Sihlahla^a, Philiswa N. Nomngongo^b, Nomvano Mketo^{a,*}

^a Department of Chemistry, College of Science and Engineering and Technology, Florida Science Campus, University of South Africa, Roodepoort, 1710, Johannesburg, South Africa

^b Department of Chemical Sciences, University of Johannesburg, PO Box 17011, Doornfontein 2028, Johannesburg, South Africa

*Corresponding author: Mketon@unisa.ac.za

Abstract

A greener sample preparation method based on magnetic solid phase microextraction (MSP μ E) was developed for the preconcentration of neonicotinoid pesticides (acetamiprid, imidacloprid, thiacloprid and thiamethoxam) in vegetable oil samples followed by separation and quantification using high performance liquid chromatography with diode array detector (HPLC-DAD). Different characterisation techniques such as Fourier Transform Infrared Spectroscopy (FTIR), Powder X-ray diffraction analysis (PXRD), Thermogravimetric Analysis (TGA), Transmission electron microscopy (TEM), and scanning electron microscope and energy-dispersive X-ray spectroscopy (SEM-EDS) confirmed the synthesised magnetic nano adsorbents (Fe_3O_4 , $\text{Fe}_3\text{O}_4@\text{Al}_2\text{O}_3$ and $\text{Fe}_3\text{O}_4@\text{Al}_2\text{O}_3/\text{AC}$). The most influential parameters affecting MSP μ E of NEOs by $\text{Fe}_3\text{O}_4@\text{Al}_2\text{O}_3/\text{AC}$ were examined using a multi-variate optimisation approach and 8 min extraction time, 13 pH, 9 mg adsorbent mass, and 0.5 mL eluent volume were optimal parameters. The proposed $\text{Fe}_3\text{O}_4@\text{Al}_2\text{O}_3/\text{AC}$ method showed high accuracy (80–119.21%) and precision ($\leq 10\%$) for all the investigated NEOs. Additionally, the obtained limit of detection (LOD) ranged from 0.5–1.76 ng. μL^{-1} , the limit of quantification (LOQ) ranged from 1.87–6.62 ng. μL^{-1} and satisfactory high pre-concentration factors (73.02–407.0) were comparable with literature reported studies. The Analytical GREENess calculator AGREE, BAGI and NEMI analysis confirmed greenness of MSP μ E. After that, the validated MSP μ E method was applied to real vegetable oil samples (avocado, canola, olive and sunflower), and fortunately, all the investigated NEOs were below LODs of the proposed MSP μ E /HPLC-DAD methods.

Keywords: Neonicotinoid pesticides; Vegetable oils Magnetic solid phase microextraction (MSP μ E) HPLC-DAD; Greenness assessment

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ELECTROSYNTHESIS OF BENZIMIDAZOLE-FUSED QUINAZOLINONES VIA A CASCADE ADDITION-DESULFURIZATION-CYCLIZATION PROCESS

Khuyen Thu Nguyen^a, Mongkol Sukwattanasinitt^a, Sumrit Wacharasindhu^{a,b,*}

^aDepartment of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

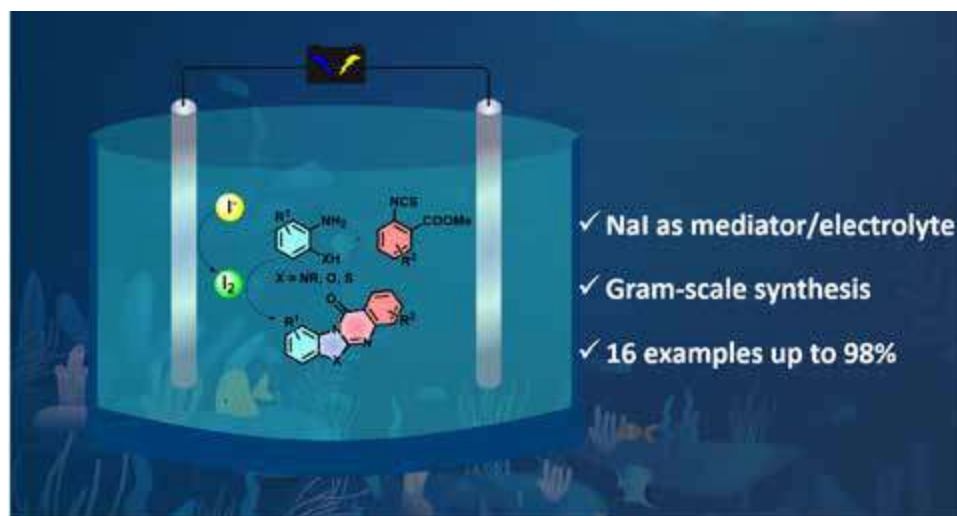
^bGreen Chemistry for Fine Chemical Productions and Environmental Remediation Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

*Corresponding author e-mail: sumrit.w@chula.ac.th

Abstract

An efficient and scalable electrochemical approach for the synthesis of benzimidazole-fused quinazolinones has been developed, utilizing *N*-substituted *o*-phenylenediamines and isothiocyanates in a cascade addition-desulfurization-cyclization process. This one-pot reaction is mediated by NaI in sub-stoichiometric amounts under open-flask conditions, serving as a mild, non-metal oxidizing agent. The method allows the preparation of a variety of benzimidazole-fused quinazolinones in moderate to excellent yields (30–98%, 10 examples). Optimized conditions also enable the synthesis of benzoxazoloquinazolinones and benzothiazoloquinazolinones, with yields ranging from 30 to 72% (6 examples). The process is scalable, maintaining high efficiency at the gram scale. Key to the high yields is the effective generation of iodine-oxidizing species at the anode and the overnight stirring of precursors to maximize thiourea intermediate formation. Notably, the approach is characterized by a simple, one-pot, three-step reaction sequence, utilizing sub-stoichiometric NaI without requiring external additives. The versatility of the method is demonstrated by its application to diverse substrates, including bioactive compounds. This electrochemical strategy presents a promising, green synthesis route for biologically active amino heterocycles, offering a sustainable alternative to traditional synthetic methods.

Keywords: Benzimidazole-fused quinazolinones, Electroorganic synthesis, Desulfurization, Cascade reaction, NaI-mediator



STUDY ON THE SELECTIVITY OF TOPO BASED DESS FOR PGMS EXTRACTION

Lingen Guo^a, Yutaro Takaya^{a,b,*}, Chiharu Tokoro^{b,a}

^aThe University of Tokyo

^bWaseda University

*Corresponding author: y-takaya@sys.t.u-tokyo.ac.jp

Abstract

Platinum group metals (PGMs) are essential for the industrial world, and in the recent years recycling has become an unignorable source for gaining PGMs (Fig.1). Recently, deep eutectic solvents (DESS; Fig.2) based on trioctylphosphine oxide (TOPO; Fig.3) have been proved to be useful for the extraction and separation of metal ions. In this study, we prepared DESS by mixing TOPO with different alcohols and examined their effectiveness in separating platinum and palladium in solutions with different salt and acid concentrations (Fig.4). Meanwhile we also analyzed the relevant physicochemical properties behind it. The detailed discussion will focus on the following points, with the aim of determining the optimal recipe for the separating of platinum and palladium using liquid-liquid extraction.

1. Effect of aqueous phase and DES phase composition
2. Chemical environment of P=O group under different conditions
3. Changes in the structure of DES after contact with aqueous phase

The results show that in the aqueous phase, acid plays a more important role in the separation of PGMs than salt. Meanwhile, in the DES phase, hydrophobic alcohols with moderate charge density on the carboxyl groups are more favorable for this work.

Keywords: selective extraction, platinum group metal separation, liquid-liquid extraction, resource and waste treatment, deep eutectic solvent

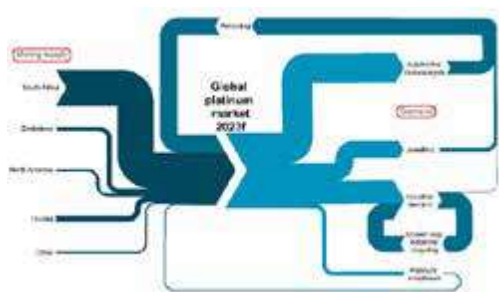


Fig.1 Producing and consumption of PGMs [1]

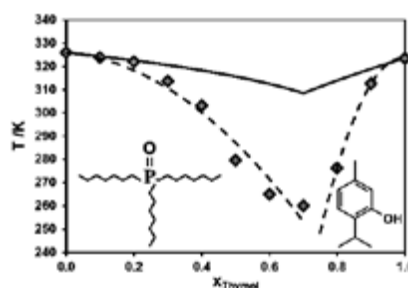


Fig.2 Non-ideality of TOPO based DES [2]



Fig.3 Structure of TOPO

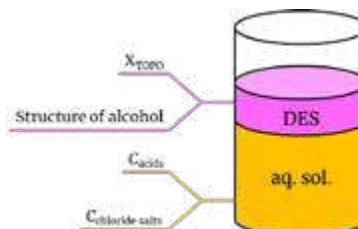


Fig.4 Condition control

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DITHIOCARBAMATE-FUNCTIONALIZED CELLULOSE FOR EFFECTIVE SEPARATION OF LEAD FROM CHELATOR-WASHED SOIL EFFLUENTS

Pranta Sarker,^{a,*} Moe Marumoto,^a Ismail M.M. Rahman,^{b,*} Kuo H. Wong,^c Asami S. Mashio,^c Tatsuya Nishimura,^c Katsuhiko Maeda,^c Hiroshi Hasegawa^{c,*}

^a Graduate School of Natural Science and Technology, Kanazawa University, Japan

^b Institute of Environmental Radioactivity, Fukushima University, Japan

^c Institute of Science and Engineering, Kanazawa University, Japan

*Corresponding author: prantasarker12@gmail.com

Abstract

The effective removal of lead (Pb) from waste streams containing chelators remains a significant challenge due to the high stability and mobility of Pb-chelator complexes. This study investigates the efficacy of a novel, cost-efficient, biomass-based sorbent, namely proline-incorporated dithiocarbamate-modified cellulose crosslinked with epoxy (DMC-Pro-Epo6), for the selective extraction of Pb(II) ions from chelator-washed soil effluents. DMC-Pro-Epo6 demonstrated remarkable Pb(II) sorption capacity under controlled conditions and in the presence of excessive chelators. Even with a 100-fold excess of chelators and competing metal ions, the sorbent maintained high removal efficiency. Furthermore, DMC-Pro-Epo6 exhibited superior separation performance compared to commercially available ion-selective sorbents. The sorption kinetics followed a pseudo-second-order model, achieving equilibrium within 20 minutes. Langmuir isotherm analysis revealed maximum sorption capacities of 1267 and 659 $\mu\text{mol g}^{-1}$ in Pb(II)-containing aqueous solutions and Pb(II)-EDTA solutions, respectively. X-ray photoelectron and absorption spectroscopy, alongside sorption parameters, confirmed that Pb(II) sorption onto DMC-Pro-Epo6 occurs via a chemisorption mechanism. Validation experiments using real waste samples with complex chelator and base metal ion matrices demonstrated a quantitative Pb(II) extraction efficiency of 92–99%. These promising results highlight the scalability of the proposed process, offering a more effective and simplified approach for separating metal ions and chelators from wastewater compared to conventional treatment methods.



Keywords: Dithiocarbamate-functionalized cellulose; Lead separation; Excess chelator; Sorptive separation; Soil washing effluent

SMALL-SCALE TITRATION AS A GREEN CHEMISTRY-BASED ALTERNATIVE: A COMPARATIVE STUDY WITH CONVENTIONAL METHODS

Marc Kye Peng Tang^{a*}, Sheau Huey Chong^b

^a*Garden International School, Malaysia*

^b*Tunku Abdul Rahman University of Management and Technology, Malaysia*

^{*}*Corresponding author: marctang08@gmail.com*

Abstract

Titration is a fundamental analytical technique, however conventional methods generate excessive chemical waste. This study applies small-scale chemistry principles¹ to strong acid-strong base titration of 0.1 M HCl against 0.1 M NaOH, evaluating accuracy and precision at reduced volumes. Comparing conventional (25.0 mL NaOH) and small-scale conditions (10.0, 5.0, 2.0, and 1.0 mL NaOH), results show that small-scale titration maintains reliability. At 5.0 mL NaOH, endpoint accuracy (6.0% deviation from expected) closely aligns with conventional titration (4.6% deviation). Accuracy decreases at 2.0 mL NaOH (20.0% deviation) and becomes unreliable at 1.0 mL NaOH (203% deviation). Findings confirm that small-scale titration is a viable alternative. 5.0 mL NaOH is the practical lower threshold, significantly reducing chemical waste whilst maintaining precision. Small-scale titration aligns with Green Chemistry and UN SDG 12², promoting sustainability in chemical analysis.

Keywords: Titration, Small-Scale Chemistry, Green Chemistry, Chemical Waste, Sustainability

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SUSTAINABLE ANALYTICAL TECHNIQUES: COMPARING SMALL-SCALE AND CONVENTIONAL UV-VIS METHODS FOR CHROMIUM (III) NITRATE ANALYSIS

Sheau Huey Chong^{a,*}, Jia Wei Wong^b

^a*Tunku Abdul Rahman University of Management and Technology.*

^b*Tunku Abdul Rahman University of Management and Technology*

**Corresponding author: chongsh@taru.edu.my*

Abstract

With growing emphasis on green chemistry, reducing reagent consumption in analytical procedures is a priority. Small-scale UV-Vis spectrophotometry offers a sustainable alternative to conventional methods. This study evaluates its accuracy in chromium (III) nitrate quantification compared to conventional techniques. This research aims to determine whether small-scale (reduced concentration) UV-Vis spectrophotometry provides equivalent analytical performance to conventional methods while minimizing chemical waste. Calibration standards were prepared at two concentration ranges and analysed at 430 nm: small-scale (0.001 M–0.005 M) and conventional (0.01 M–0.05 M). Absorbance readings were obtained, and calibration curves were constructed. To test the lower detection limit, an additional small-scale range (0.0001 M–0.0005 M) was analysed. The small-scale method demonstrated high accuracy, yielding an r^2 of 0.998, closely matching the conventional method ($r^2 = 0.9997$). This confirms its potential as a low-waste alternative. However, at concentrations below 0.0005 M, the linearity decreased significantly ($r^2 = 0.8702$), indicating reduced sensitivity. Potential causes include increased noise-to-signal ratio and limitations in detection at very low absorbance levels. Small-scale UV-Vis spectrophotometry provides a reliable and sustainable approach for chromium (III) nitrate determination at standard concentrations. However, it is less effective at trace levels. Future improvements, such as using more sensitive cuvettes or alternative wavelength selections, could enhance its detection capabilities.

Keywords: Micro-scale, Sustainable Development Goal 12 (SDG 12), Sustainability in chemistry

ADSORPTION OF HEAVY METALS FROM ACID MINE DRAINAGE USING POLY (HYDROXAMIC ACID) LIGAND NOZIPHO NOMPUMELELO MABASO

Nozipho Mabaso

Biosorption and Water Research Laboratory, Department of Natural Sciences, Vaal University of Technology, P. Bag X021, Vanderbijlpark, 1900, South Africa
Corresponding author: noziphom@vut.ac.za

Abstract

Acid mine drainage (AMD) poses severe environmental concerns due to its high acidity, toxic metals, and sulphate content. Conventional treatment methods are often ineffective, highlighting the need for cost-effective remediation technologies. This study explores AMD remediation using a modified pine cone powder biosorbent. The biosorbent surface was enhanced through Fenton reagent pretreatment and chemically grafted with acrylic acid via free radical initiation. The modified adsorbent was tested for Fe^{3+} , Cu^{2+} , Mn^{2+} , Zn^{2+} , and Pb^{2+} removal from single-component solutions and AMD samples from an abandoned mine in Witbank. The adsorption behaviour of the poly (hydroxamic acid) ligand was assessed to determine its suitability for AMD treatment. Batch experiments were conducted to evaluate adsorption rates and equilibrium uptake in single and multi-component solutions. The optimal pH for heavy metal ion removal was 6, with percentage removals of 79% (Fe^{3+}), 83% (Cu^{2+}), 82% (Mn^{2+}), 90% (Zn^{2+}), and 73% (Pb^{2+}). The ligand's binding capacities (q_e , mg g^{-1}) were 13 (Fe^{3+}), 14 (Cu^{2+}), 11 (Mn^{2+}), 11 (Zn^{2+}), and 12 (Pb^{2+}). Adsorption data fitted well with the Langmuir isotherm model ($R^2 > 0.999$), indicating monolayer adsorption. Additionally, R_L values (0.0020–0.0560) confirmed favourable adsorption. Pseudo-second-order kinetics best described adsorption behaviour, suggesting chemisorption. Overall, poly (hydroxamic acid) ligand demonstrated strong potential as a low-cost and efficient material for AMD treatment.

Keywords: Acid mine drainage, Grafting, Poly (hydroxamic acid) ligand, Heavy metals, Adsorption

PINECONE-DERIVED ADSORPTIVE BIO-NANOCOMPOSITES AS ENHANCERS FOR MONO- AND CO-DOPED AMORPHOUS TiO_2 IN WASTEWATER REMEDIATION APPLICATIONS

Kgomotso N.G. Mtshatsheni^{a*}, Sithembela A. Zikalala^b, Eliazer B. Naidoo^a, Edward N. Nxumalo^b

^a*Department of Chemistry, Vaal University of Technology, Private Bag X 021, Vanderbijlpark, 1900, South Africa*

^b*Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida, 1709, Johannesburg, South Africa*

**Corresponding author: kgomotsom@vut.ac.za*

Abstract

The growing issue of water scarcity underscores the need for more efficient water treatment technologies. Conventional wastewater treatment often fails to remove a broad range of pollutants, particularly dyes from industries. Photocatalysis and adsorption have emerged as promising techniques for removing these dyes. This study developed pinecone-derived photocatalytic and adsorptive bio-nanocomposites for dye removal. The approach involved doping and compositing TiO_2 to reduce crystallinity, using a simple sol-gel process to design TiO_2 nanocomposites for textile dye degradation. The process included a slurry of repurposed plant-based adsorbents, such as unmodified pinecone and magnetite (PMC) composites, as well as modified composites grafted with polyacrylic acid (GAA).

The freshly synthesized composites, including TiO_2 -GAA, TiO_2 -PMC, and control photocatalysts (TiO_2 and NTiO_2), were extracted through drying and heating. All the photocatalytic composites were confirmed to be amorphous, with N-doping affecting the morphology and surface properties. N-doped photocatalysts exhibited smaller particle sizes and higher surface areas. Compositing with adsorbents reduced the indirect energy band gap, enabling these composites to absorb more in the UV region while showing improved photosensitivity in the visible range. The photocatalytic performance was tested under UV light using a dye mixture of reactive red 120 (RR 120) and rhodamine B (RhB) at 25 ppm concentration, with pH adjusted to 8, simulating typical textile wastewater.

The degradation rates of the N-doped photocatalysts followed pseudo-zero-order kinetics, while others followed pseudo-first-order kinetics. GAA-based nanocomposites and TiO_2 exhibited the highest dye removal efficiency. This study highlights the effectiveness of acrylic acid-grafted, repurposed adsorbents in modifying photocatalysts to achieve performance comparable to highly crystalline doped TiO_2 , offering a greener alternative for wastewater treatment.

Keywords: Photocatalyst, bio-nanocomposite, amorphous TiO_2 , pinecone

SYNTHESIS OF MAGNETITE (Fe₃O₄) NANOPARTICLES FUNCTIONALISED WITH CYCLODEXTRIN VIA POLYDOPAMINE COATING FOR THE REMEDIATION OF TETRACYCLINE AND CIPROFLOXACIN FROM AQUEOUS SOLUTION

Agnes Pholosi^a, Emmanuel Adisa^a, Samson Akpotu^a, Vusumzi Pakade^b

^aBiosorption and Water Treatment Research Laboratory, Vaal University of Technology, Private Bag X021, Vanderbijlpark, 1900, South Africa

^bDepartment of Chemistry, College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, 1710, South Africa

*Corresponding author: agnesp@vut.ac.za

Abstract

Advancements in nanotechnology and increments in the knowledge of synthesis and characterization of varieties of nanoparticles birthed the development of hybrid nano adsorbents. Magnetic nanoparticles exhibit high surface area, tunable surface properties and unique magnetic properties¹ while polysaccharide materials have exceptional structure and unique properties². To explore this potentials, magnetic nanocomposite was synthesized by coating magnetite with silica (SiO₂) using the modified Stober route. The synthesized Fe₃O₄-SiO₂ was polymerized with dopamine in a basic solution to obtain Fe₃O₄-SiO₂-PDA followed by functionalization with β-cyclodextrin. The successful synthesis of Fe₃O₄-SiO₂-PDA-CD nanocomposite was confirmed through scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared (FTIR), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). Batch adsorption studies were conducted to investigate if the synthesized nanocomposite could adsorb tetracycline (TC) and ciprofloxacin (CIP) from aqueous solution. Functionalization of magnetite with polydopamine and cyclodextrin led to improvement in surface characteristics and incorporation of relevant functional groups. XRD results showed that magnetite retained its magnetic properties after incorporation of PDA and CD. Morphological and structural analysis showed the presence of iron, carbon, oxygen, and nitrogen with spherically shaped nanoparticles with average particle size of 12.02 nm. Maximum adsorption was achieved at pH 7 and equilibrium time was reached before 30 min for initial concentration ranging from 50 to 300 mg/dm³. The adsorption kinetics suited pseudo second order model and equilibrium data fitted Langmuir isotherm with TC and CIP adsorption capacity of 286.13 and 446.56 mg/g, respectively. These findings highlight the strong potential of Fe₃O₄-SiO₂-PDA-CD nanocomposite as an effective adsorbent for TC and CIP remediation in contaminated wastewater

Keywords: Cyclodextrin, Kinetics, Magnetic nanocomposites, Water remediation, adsorption

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SYNTHESIS, EVALUATION AS HERBICIDES AND ECOTOXICITY OF NEW CYCLOPEPTIDES WITH INHIBITORY ACTIVITY ON CYANOBACTERIA

Gloria Serraa*, Camila Irabuena^a, Laura Posada^a, Lucila González^b, Luciana Rey^c, Melanie Silva^c,
 Lucia Boccardi^d, Luis Aubriot^b, Juana Villalba^c, Diana Miguez^d, Laura Scarone^a

^aLaboratorio de Química Farmacéutica, DQO, Facultad de Química, Udelar, Montevideo, Uruguay. ²Limnología, Facultad de Ciencias, Udelar, Montevideo, Uruguay.

^cLaboratorio de Malezas, EEMAC, Facultad de Agronomía, Udelar, Paysandú, Uruguay.

^dLatitud, Avenida Italia 6201, Montevideo, Uruguay

*Corresponding author: gserra@fq.edu.uy

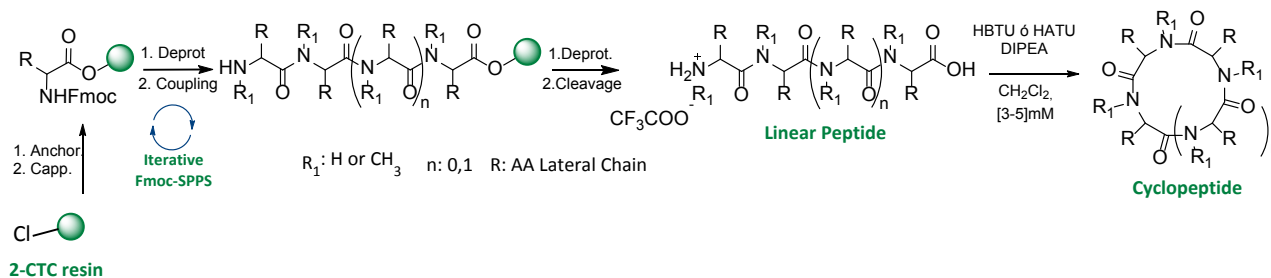
Abstract

The intensive use of synthetic herbicides during the last 50 years has led to environmental and ecological impact.¹ These agricultural practices, several hydrological alterations and the global warming promote cyanobacteria blooms, which have increased globally during recent years in intensity, frequency and duration.² In addition, as the effectiveness of the commercially available herbicides is decreasing, the development of new ones is of great importance. Products originated from living organisms and natural metabolites, have emerged as an alternative for sustainable agriculture. A significant number of natural products derived from amino acids, among them, cyclopeptides, have been described with herbicidal, fungicidal or insecticidal activity.

The objective of our investigations,³ is to develop cyclopeptides as potential ecofriendly herbicides and inhibitors of cyanobacteria.

In this work, we present the synthesis of peptides by Solid Phase Peptides Synthesis using Fmoc strategy and the solution macrocyclization to obtain tetra- and penta-cyclopeptides. In addition, the herbicidal evaluation in crops and their corresponding weeds, the activity against Cyanobacteria and eucariotic alga, and studies of ecotoxicity using *Daphnia* and Microtox® test will be presented.

Keywords: cyclopeptides, herbicides, ecofriendly, synthesis.



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HIGHLY EFFICIENT CATALYTIC PREPARATION OF BIO JET-FUEL PRECURSORS BY AMINO-FUNCTIONALIZED BASIC γ - Al_2O_3

Suya Yin^{a,b}, Xujing Tang^{a,b}, Yuanyuan Wang^{a,b*}.

^aState Key Laboratory of Petroleum Molecular & Process Engineering, East China Normal University, No. 500 Dongchuan Road, Shanghai 200241, PR China

^bShanghai Key Laboratory of Green Chemistry and Chemical Processes, East China Normal University, Shanghai 200062, PR China

*Corresponding author: yywang@chem.ecnu.edu.cn

Abstract

The synthesis of bio jet-fuel precursors from biomass platform compounds through aldol condensation is a crucial step in the production of aviation liquid fuels.¹ However, current research is still restricted by several pressing issues, such as the selection of raw materials, the leaching of catalytic active sites, and catalyst deactivation.² We aim to develop an amino-grafted SA_{10} -6TES catalyst for the aldol condensation of furfural and acetone, which are biomass platform compounds, to prepare bio jet-fuel precursors. And we will focus on the following points:

1. The structure of the catalyst as characterized by spectroscopic and microscopic techniques.
2. The catalytic performance of the catalyst in the aldol condensation of furfural and acetone.
3. The reaction mechanism of C–C bond formation.

The results show that the synergistic effect between silanol groups and stable and highly efficient Lewis - base active sites has a positive promoting effect on the formation of C–C bonds between furfural and acetone, enabling almost complete conversion of furfural and giving the catalyst an excellent turnover rate. Under the optimal conditions of 333 K, 2 h and a molar ratio of furfural to acetone of 1:5, the catalyst achieved a furfural conversion rate of 99.6% and a total selectivity for condensation products of 96.6%. Moreover, it still maintained a high conversion rate after multiple cycles.

Keywords: γ - Al_2O_3 ; furfural; aldol condensation; bio jet-fuel

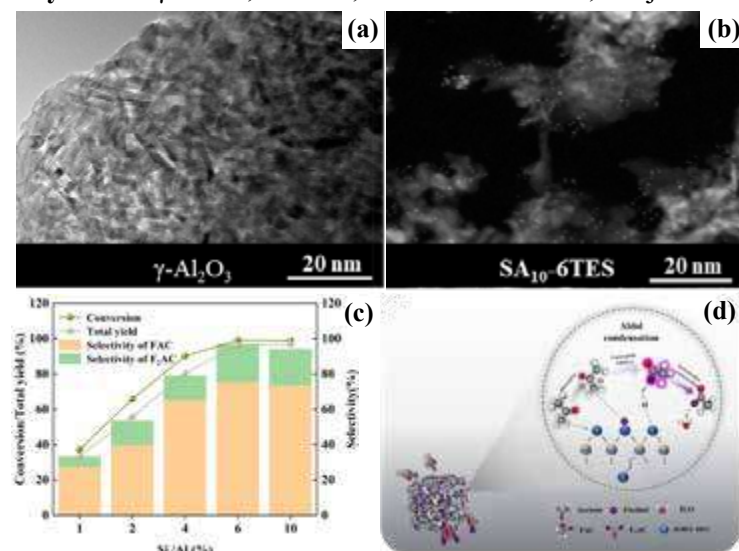


Fig. 1 (a, b) TEM images of γ - Al_2O_3 and SA_{10} -6TES; (c) The influence of amino grafting on the conversion and yield; (d) The possible reaction mechanism of SA_{10} -6TES.

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INVESTIGATION OF THE EFFECTIVENESS OF FOOD GRADE REAGENTS IN THE EXTRACTION OF CELLULOSIC PLANT FIBERS

Jennifer Bandao-Antonio

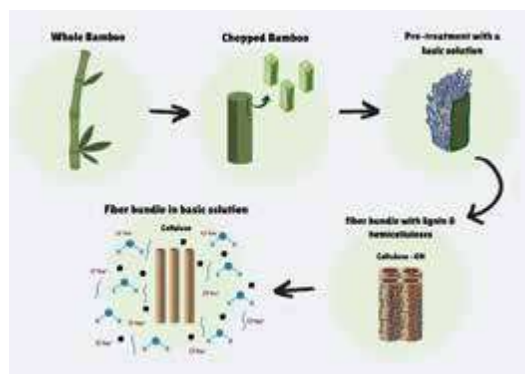
University of the Philippines Baguio, Governor Pack Road, Military Cut-Off, Baguio City Philippines 2600

Corresponding author: jbantonio4@up.edu.ph

Abstract

Food grade reagents are cheap, readily available, safer to work on, and non-toxic to living organisms and to the environment. Their effectiveness in the extraction of cellulosic plant fibers help reduce the use of inorganic reagents which are often employed in chemical treatment methods to produce fiber strands with improved surface topography and crystallographic structures. It is the aim of my investigation to determine the effectiveness of sodium bicarbonate (NaHCO_3)/baking soda, acetic acid (CH_3COOH) in white vinegar, and H_2O_2 in the production of cellulosic fibers from banana (*Musa acuminata*) pseudo-stem and sayote (*Sechium edule*) vines. Plant samples were collected and sun-dried before chemical pre-treatment for 6 days and 10 days. Pre-soaked samples were then mechanically crushed, acid hydrolyzed, and treated with H_2O_2 . The samples were washed with distilled water every after chemical treatment. Characterization techniques such as XRD analysis, Digital Microscopy, Scanning Electron Microscopy, and FTIR analysis were employed to determine Crystallinity Index (CI), fiber fineness, surface morphology, and chemical properties of the extracted cellulosic fibers. I found out that longer pre-soaking time produced fibers with higher CI, finer strands, smooth and organized fiber surface, and decreased surface impurities. This study therefore proves the effectiveness of food grade reagents in the production of cellulosic fibers from plants. These cellulosic fibers can be employed in eco-friendly composite fabrication, water filtration devices, textiles, and among other applications.

Keywords: Cellulosic Fibers, Food Grade Reagents, Eco-friendly composites, Sayote Fibers, Banana Fibers



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CHARATERIZATION OF GREEN SUPRMOLECULAR SOLVENTS AND THEIR POTENTIAL AS EXTRACTION SOLVENTS IN BIOREFINERY

María González-Miquel*, Andrea Sánchez-Monedero, Ismael Díaz, Manuel Rodríguez

Dpto. Ingeniería Química Industrial y del Medio Ambiente, ETSI Industriales, Universidad Politécnica de Madrid, C/ José Gutiérrez Abascal 2, Madrid, 28006, Spain

**Corresponding author: maria.gonzalezmiquel@upm.es*

Abstract

Supramolecular solvents (SUPRAS) are a new generation of green solvents defined as nanostructured liquids composed by colloidal suspensions of amphiphiles formed by self-aggregation and coacervation processes. These solvents are receiving increasing attention as efficient and environmentally friendly alternatives to conventional organic solvents in extraction processes, due to their capacity to capture specific solutes in their supramolecular environment.¹

The objective of this study is to propose a variety of green SUPRAS composed of ethanol, water, and organic acids or natural eutectic solvents (NAES), to perform their physico-chemical and structural characterization, and to assess their efficiency as extraction solvents of natural antioxidants from lignocellulosic biomass.

In particular, the SUPRAS used herein were prepared using ethanol, water, and five different amphiphiles (two organic acids: octanoic acid and decanoic acid; and three NAES: octanoic acid: decanoic acid [1:1], menthol: octanoic acid [1:1], and menthol: decanoic acid [1:1]). All SUPRAS were characterized in terms of their chemical compositions of the equilibrium phases, polarity, phase ratios, and phase diagrams of the ternary systems. In addition, Scanning Electron Microscopy (SEM) studies were also performed to demonstrate the unique microstructures of the proposed SUPRAS. Finally, the SUPRAS were tested as extraction solvents for the recovery of antioxidants from olive leaves and the stability of the antioxidant extracts was evaluated, with octanoic acid-based SUPRAS being the most effective extraction solvent while providing a suitable medium to preserve the stability of the antioxidants over time. Overall, this work demonstrates the potential of SUPRAS as sustainable solvents for biomass valorisation purposes in the biorefinery context.²

Keywords: Supramolecular solvents, characterization, extraction, antioxidants, biorefinery.

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FUNCTIONALIZATION OF BIOFILMS WITH ANTIOXIDANT EXTRACTS FROM OLIVE LEAVES USING GLYCEROL-BASED GREEN SOLVENTS

Emilio J. González*, Andrea Sánchez-Monedero, Ana Lafuente, Jaime Tiemblo, Marina P. Arrieta.

Dpto. Ingeniería Química Industrial y del Medio Ambiente, ETSI Industriales, Universidad Politécnica de Madrid,

C/ José Gutiérrez Abascal 2, Madrid, 28006, Spain

**Corresponding author: ej.gonzalez@upm.es*

Abstract

The fabrication of biofilms based on Poly (lactic acid) (PLA) with antioxidant properties represents an important advancement in the development of sustainable and functional materials. PLA, a biodegradable polymer, is a promising alternative to petrochemical plastics, with applications in packaging, agriculture, medicine, textiles, and automotive industries¹. Incorporating antioxidants into biofilms reduces free radical damage, improving product quality and shelf life, while natural compounds and sustainable methods support environmental protection and the circular economy.

This study presents an innovative and sustainable approach for the development of antioxidant PLA-based biopolymers by incorporating bioactive compounds derived from olive leaves. Specifically, the methodology involves two main stages: (1) the extraction of antioxidant compounds using glycerol and glycerol-based eutectic mixtures (proline, chloride choline, or betaine + glycerol (1:2)); and (2) the incorporation of these extracts into a biobased and biodegradable polymeric matrix, which allows the fabrication of biofilms with enhanced antioxidant properties. In the first case, the extractions were performed under previously optimized conditions (30 minutes, 60 °C, 900 rpm, and 1:10 S:L ratio), and the potential of the extracts was assessed in terms of antioxidant capacity and total phenolic content. On the other hand, the functionalized PLA-based films were fabricated by melt extrusion and subsequently processed into films through compression molding. Furthermore, their thermal and mechanical properties were evaluated for characterization.

Preliminary results show that olive leaf extracts enhance biofilms with antioxidant properties, improved flexibility, and sustainability, adding value to agricultural by-products. These enriched biofilms present eco-friendly alternatives for food and packaging, supporting a circular economy.

Keywords: functionalized biofilms, characterization, extraction, antioxidants, deep eutectic solvents

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RAPID SYNTHESIS OF METAL-ORGANIC FRAMEWORK

Rachel Yie Hang Tan^a, Choy Sin Lee^{b,*}, Shew Fung Wong^c, Yun Khoon Liew^d

^a*Centre of Postgraduate Studies, IMU University, 57000 Kuala Lumpur, Malaysia.*

^b*Department of Pharmaceutical Chemistry, School of Pharmacy, IMU University, 57000 Kuala Lumpur, Malaysia.*

^c*Centre of Environmental and Population Health, Institute for Research, Development, and Innovation, IMU University, 57000 Kuala Lumpur, Malaysia.*

^d*Department of Life Sciences, School of Pharmacy, IMU University, 57000 Kuala Lumpur, Malaysia.*

**Corresponding author: choysin_lee@imu.edu.my*

Abstract

Metal-organic frameworks (MOFs) are a class of inorganic-organic coordination polymers consisting of metal ions coordinated to organic linkers forming one-, two-, and three-dimensional structures. Their excellent properties, including well-defined pores, high crystallinity, and the ability to encapsulate and release drugs, analytes, and other bioactive molecules, make them highly attractive in biomedical fields such as oncology therapy, biosensing, biological imaging, and wound healing. However, commercial MOFs such as HKUST-1, ZIF-8, UiO-66, and MIL-101 are synthesised using aromatic groups and aromatic heterocyclic linkers, whose π -system contribute to poor biodegradability, structural rigidity, and potential toxicity. Additionally, the most commonly used synthesis method, hydrothermal reaction, requires prolonged reaction times of at least 12 hours. In this work, zinc salt and aliphatic organic linkers were used to synthesise Zn-MOF via a microwave-assisted method, reducing the reaction time to 1 hour for a more efficient and sustainable synthesis. The synthesised Zn-MOF was characterised by FT-IR spectroscopy, powder X-ray diffraction, and thermogravimetric analysis by TG-DTA. The disappearance of characteristic peaks of the carboxyl group at 1689-1707 cm^{-1} indicates the linkers have been completely deprotonated and have formed coordination with zinc ions to form Zn-MOF, which have shown new peaks at 1527, 1458, and 1396 cm^{-1} , corresponding to -COO^- carboxylate stretching peak. The PXRD results have proven the high crystallinity of Zn-MOF. Furthermore, the Zn-MOF was subjected to *in vitro* hemolytic assay to determine its hemocompatibility. The newly synthesised Zn-MOF exhibited a lower hemolysis rate compared to the commercial MOF (ZIF-8 and Zn-BTC), indicating its superior hemocompatibility and potential applications in medical devices or blood contacting materials.

Keywords: Metal-organic framework, XRD, FT-IR, hemocompatibility

ELECTROGENERATED BASE DRIVEN TRANSFER HYDROGENATION REACTION OF AROMATIC KETONES

Huan Wang^{a,*}, Hao Xu^a, Haihong Wu^a, Jiaying Lu^a

^aKey Laboratory of Petroleum Molecular & Process Engineering, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai 200062, China

*Corresponding author: hwang@chem.ecnu.edu.cn

Abstract

As a basic chemical, aromatic alcohol is also the precursor of many high-value chemicals, which plays a vital role in drug synthesis, spices and cosmetics, agricultural applications, environmental protection and green chemistry. Under mild conditions, the efficient transfer hydrogenation of aromatic ketones to synthesis aromatic alcohols with high selectivity can be achieved using alcohols as solvents, hydrogen sources, and precursors of bases, driven by electrogenerated bases in a metal-complex catalytic system.[1] Moreover, solvents have a significant impact on the reaction. In *i*-PrOH, the metal complex catalyst undergoes a similar reaction process to that driven by conventional organic bases, which promotes substrate hydrogenation through the synergistic promotion of the ligand and the metal center to give alcohols with moderate ee values. In contrast, in MeOH, electrochemistry can drive the transfer hydrogenation reaction, which is challenging for conventional organic bases, under mild conditions to obtain racemic alcohols.[2]

Keywords: Electrogenerated base, transfer hydrogenation, aromatic ketones, aromatic alcohols



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NEAR INFRARED REFLECTANCE SPECTROSCOPY (NIRS) FOR SIMULTANEOUS EVALUATION OF SOIL PROPERTIES

Syazwani binti Bakar^{a*}, Irna Syairina binti Sahari^a, Margaret anak Abat^a

^aAgriculture Research Centre Semongok, Department of Agriculture Sarawak KM 20, Borneo Heights Road, 93250 Kuching, Sarawak, Malaysia.

*Corresponding author: syazwanib@sarawak.gov.my

Abstract

The conventional methods for soil analyses are often time consuming, and pose potential risk hazards. Near-infrared reflectance spectroscopy (NIRS) has gained attention for measuring soil constituents because it is rapid, non-destructive and perhaps cost efficient. However, NIRS technology has not been widely adopted locally for soil quality study and monitoring. To our knowledge, limited reports were published about NIRS technology to predict soil properties. Therefore, the objective of this study was to evaluate the potential of NIRS in predicting soil properties of Sarawak. A total of 165 mineral soils were scanned to obtain their NIR spectrum in the wavelength ranging from 400 nm to 2500 nm. Calibration and prediction models were developed using NIRS to predict soil texture (clay, silt, fine and coarse sand), total nitrogen, cation exchange capacity, exchangeable cations, total organic carbon, available phosphorus, pH and conductivity. A modified partial least squares regression with cross-validation analysis was carried out using the calibration set and the resulting model prediction ability was established using the prediction set. The absorbance bands of the selected samples were broad with peaks overlapping across the infrared wavelength due to the complex compositions in the soil samples (*Figure 1a*). The first order derivative (*Figure 1b*) were obtained using the selected mathematical treatments.

Except for soil texture analyses, the NIRS technique demonstrated an excellent laboratory prediction performance with regression coefficients (R^2_{val}) between 0.825 and 0.991, and ratio of prediction deviation (RPD) between 2.129 and 9.438, in agreement with published findings¹. Soil texture predictions were less accurate than the laboratory results, with RPD values between 0.457 and 1.006. Statistics paired t-test also showed reasonable similarities between measured and predicted values for all models. Future study will include the improvement to the calibration models for soil texture analyses and application on different soil types.

Keywords: non-destructive, simultaneous, soil, sustainable agriculture

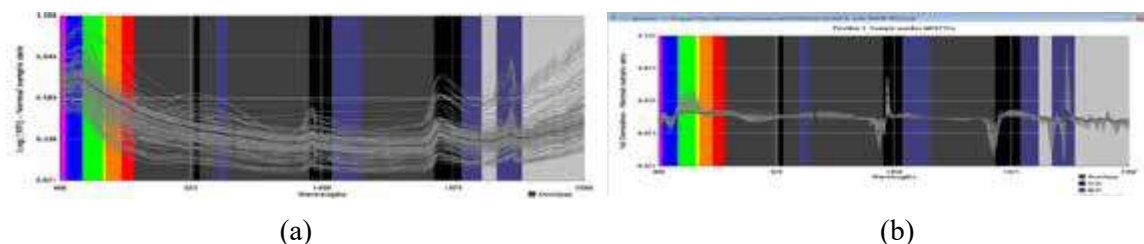


Figure 1. (a) Spectral absorption scanned by NIRS showed the variation in soil analysis; (b) The first derivative (D1) of spectral absorption calculated using mathematical treatments and scattering methods.

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ZN-MOFS: SYNTHESIS, CHARACTERISATION AND HEMOCOMPATIBILITY TEST

Bing Wei Chua^a, Choy Sin Lee^{b,*}, Mallikarjuna Rao Pichika^b, Wen Huei Lim^c

^aCenter of Postgraduate Studies, IMU University, Malaysia.

^bDepartment of Pharmaceutical Chemistry, School of Pharmacy, IMU University, Malaysia.

^cAdvanced Oleochemical Technology Division, Malaysian Palm Oil Board, Malaysia.

*Corresponding author: choysin_lee@imu.edu.my

Abstract

Metal organic frameworks (MOFs) are a class of materials formed through coordination bonds between organic linkers and inorganic metals. Their unique properties, including exceptionally high specific surface area, porosity, and tunable structures, have made them increasingly attractive for a wide range of applications, such as gas storage and separation, heterocatalysts, photosensing, and drug delivery. In the field of drug delivery, MOFs are emerging as a promising alternative to conventional drug carriers such as microparticles and micelles. This is due to MOFs having diverse morphologies and chemical properties, stable physicochemical properties upon modification, significantly larger surface area, and biodegradability thanks to weak coordination bonds. In this work, a series of Zn-MOFs were synthesised by using microwave-assisted synthesis method using linkers synthesised from palm oil-derived oleochemicals. FTIR analysis confirmed the coordination between the linker and zinc salt, as evidenced by the disappearance of peak at 1676 cm⁻¹ corresponding to carbonyl stretch of carboxylic acid, and appearance of peak at 1560 cm⁻¹ and 1369 cm⁻¹ corresponding to asymmetric and symmetric COO⁻ vibration. XRD pattern showed sharp characteristic peaks, suggesting high crystalline nature. The hemolysis assay exhibited great blood compatibility, with treatment concentration of 2000 µg/mL showing less than 4% hemolysis, compared to ZIF-8 with concentration of 1000 µg/mL showing 33% hemolysis [1]. The Zn-MOF will be evaluated as a potential drug carrier for the controlled-release of an oncology drug.

Keywords Metal Organic Framework, microwave synthesis, oleochemical, hemolysis

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SYNTHESIS OF BIO POLYOLS FOR RIGIT SANDWICH PANEL APPLICATIONS

Bilgehan Güzel^{a,*}, Orhan Kahveci^b, Sinem Tümükb, Erdem Delil^b,

^a*Çukurova University, Department of Chemistry, 01330 Adana, Turkey*

^b*TEKNOPANEL Tarsus-Mersin OSB Mersin, Turkey*

**Corresponding author: bilgehan@cu.edu.tr*

Abstract

Research on the use of bio-based renewable resources for the production of useful chemicals and new materials are rapidly increasing. The environmental compatibility and low cost of bio-based resources compared to widely used petrochemical derivatives further increase the interest in these studies, polyol, which is a polyhydroxy compound, is used in construction, coating materials, adhesives, sealants, elastomers, resins, etc. It is an important building block of polyurethanes with a wide range of applications, Polyols are traditionally produced from petroleum and are a technological product that requires a lot of energy to produce and has high costs and also has negative effects on the environment. In line with the green deal, the search for limiting petroleum-based production and reducing CO₂ emissions has led researchers to seek renewable, less costly and more environmentally friendly alternative, non-petroleum-based polyol sources. The synthesis of bio-polyols by adding hydroxyl groups to vegetable oils such as sunflower, corn, olive, palm and soybean oils is an environmentally friendly alternative and is attracting considerable attention today. In roof and facade panels, which are one of the most important application areas of the polyurethane sector, the insulating material inside the panel consists of rigid polyurethane foam.

In this project, polyol was prepared from soybean oil and its use instead of petroleum-derived polyol in rigid polyurethane foam preparation was investigated. In the studies conducted, epoxide soybean oil was added to different proportions of hydroxyl groups, the effects of hydroxyl number on foam formation and mechanical resistance of the foam were investigated. The polyol ratio in this material prepared with polyol and isopynurate is around 50% and petroleum-derived polyol is currently used. The relationship between hydroxyl numbers of the prepared polyols and rigid polyurethane foam formation performances was investigated, synthesized polyols were characterized by spectroscopic techniques such as FTIR and NMR. The morphologies of the prepared panels were examined by SEM, and their tensile, compression and stretching properties were investigated.

Keywords: Epoxidation, polyol, soybean oil, rigid polyurethane, sandwich panel

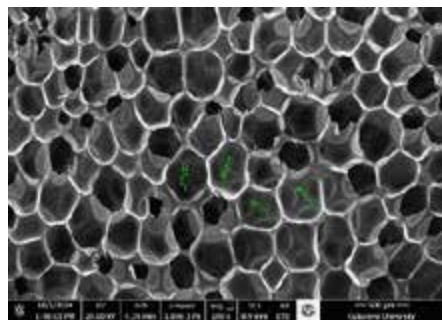


Figure: SEM image of rigid polyurethane foam

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DIRECT GROWTH AND POST-TREATMENTS OF ZIF-67 ON CARBON PAPER FOR HIGH-PERFORMANCE ELECTROCATALYSIS

Anh Ngoc Nguyen^a and Hyojong Yoo^{a*}

^a*Department of Battery and Chemical Engineering, Hanyang University ERICA, Ansan, Gyeonggi-do, 15588, Republic of Korea*

**Corresponding author: hjhaha73@hanyang.ac.kr*

Abstract

Nano metal-organic framework (NMOF)-derived transition metal chalcogenides (TMCs) offer superior electrocatalytic activity and durability. To overcome the limitations of immobilizing catalysts onto the working electrode substrate using binders, a more effective strategy is the direct growth of NMOF-derived TMC catalysts on a conductive substrate. This approach enhances electrode durability and performance. Here, we present a facile method for growing cobalt-based ZIF-67 on electrodeposited cobalt or nickel-cobalt hydroxide layers on carbon paper (CP). ZIF-67 was then transformed into (1) amorphous cobalt sulfide (Co_xS_y) to form $\text{Co}_x\text{S}_y@\text{Co}(\text{OH})_2/\text{CP}$ ($\text{CS}@\text{CH}/\text{CP}$)¹ via thioacetamide etching and (2) selenium-doped nickel-cobalt hybrids ($\text{Se-Ni}|\text{Co}/\text{CP}$)² via selenous acid etching and pyrolysis. These CP-based electrodes exhibit remarkable and durable OER, HER, and overall water-splitting performance. $\text{CS}@\text{CH}/\text{CP}$ achieves an OER overpotential of 180 mV at 10 mA cm⁻², while $\text{Se-Ni}|\text{Co}/\text{CP}$ demonstrates exceptional HER, OER, and water-splitting activity. The enhanced performance is attributed to the MOF-derived hierarchical structure, providing high porosity, abundant active sites, optimized adsorption energy, and robust self-supported construction.

Keywords: ZIF-67, transition metal-based catalyst, oxygen evolution reaction, hydrogen evolution reaction, overall water-splitting

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ZINC-BASED COORDINATION POLYMER PARTICLE-DERIVED BIMETAL-NITROGEN-CARBON FOR RECHARGEABLE ZINC-AIR BATTERY

Chaeyeon Kang^a and Hyojong Yoo^{a*}

^a*Department of Battery and Chemical Engineering, Hanyang University ERICA, Ansan, Gyeonggi-do, 15588, Republic of Korea*

**Corresponding author: hjhaha73@hanyang.ac.kr*

Abstract

Rechargeable zinc-air batteries (ZABs) hold great potential for next-generation energy storage, but their efficiency is hindered by the sluggish oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). While noble metal catalysts (e.g., Pt, Ir, and Ru) exhibit excellent catalytic performance, their high cost and poor long-term stability limit commercial viability. Transition metal-based electrocatalysts, particularly metal-nitrogen-carbon (M-N/C) systems, have emerged as promising alternatives. Among these, Zeolitic Imidazolate Framework-8 (ZIF-8) serves as an ideal template for M-N/C catalyst synthesis due to its high surface area, porosity, and nitrogen content. However, its highly crystalline nature restricts metal binding, leading to metal-carbide (M-C) cluster formation that reduces catalytic efficiency.¹ Herein, we report an effective strategy to enhance metal incorporation in ZIF-8 by introducing N_{imino}-N_{pyridine}-N_{imino} metal-binding sites via the 2,6-bis[1-(4-carboxyphenylimino)ethyl]pyridine (BCPIP) ligand. The resulting iron-nickel dual-doped Zn-based coordination polymer particles (FeNi_ZnCPP) were pyrolyzed to obtain the FeNi-NC_{CPP} electrocatalyst, which exhibited outstanding bifunctional activity. FeNi-NC_{CPP} showed remarkable OER and ORR catalytic activity, outperforming conventional noble metal catalysts. Furthermore, when applied in a rechargeable ZAB, FeNi-NC_{CPP} demonstrated a peak power density of 250 mW cm⁻² and excellent charge-discharge stability, proving its potential as a cost-effective and durable alternative for next-generation ZABs.

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HIGH-CAPACITANCE SUPERCAPACITOR ELECTRODES BASED ON NICOAL-LDH/GRAPHENE AEROGEL

Yebin Park^a and Hyojong Yoo^{a*}

^a*Department of Battery and Chemical Engineering, Hanyang University ERICA, Ansan, Gyeonggi-do, 15588, Republic of Korea*

**Corresponding author: hjhaha73@hanyang.ac.kr*

Abstract

Optimizing electrode materials is crucial for improving the energy storage performance of supercapacitors. Layered double hydroxides (LDHs) are promising due to their high theoretical capacitance, but they suffer from poor conductivity and limited ion transport. This study aims to develop a high-performance electrode by combining the advantages of LDHs with a conductive and porous framework to overcome these intrinsic limitations. A composite electrode was fabricated by electrodepositing NiCoAl-LDH onto a graphene aerogel (GA) scaffold. GA, known for its high conductivity and three-dimensional porous structure, was used to enhance electron mobility and ion diffusion. Each metal ion in the LDH plays a specific role: Ni contributes to redox activity, Co improves electrical conductivity, and Al enhances structural stability. The GA–NiCoAl LDH electrode demonstrated significantly enhanced electrochemical performance, with a specific capacitance of 2065 F/g. The interconnected structure of GA improved charge transport and mitigated the limitations of the LDH layer. These results highlight an effective synergy between the GA framework and the LDH material. The integration of NiCoAl-LDH with a graphene aerogel framework effectively addresses the shortcomings of conventional LDH electrodes. This strategy offers a viable pathway to develop high-performance supercapacitor electrodes through structural and compositional optimization.

Keywords: Supercapacitor, Layered double hydroxide, Graphene aerogel, Electrode

GOLD NANOPARTICLES DECORATED GRAPHENE AEROGEL FOR AN EXCELLENT GLUCOSE-OXIDASE-LIKE CATALYTIC AND STABLE ELECTRODE OF GLUCOSE BIOFUEL CELLS

Doan Cao Thang^a and Hyojong Yoo^{a*}

^a*Department of Battery and Chemical Engineering, Hanyang University ERICA, Ansan, Gyeonggi-do, 15588, Republic of Korea*

**Corresponding author: hjhaha73@hanyang.ac.kr*

Abstract

Glucose biofuel cells (GBFCs) offer a promising approach for directly generating energy from blood to power implanted medical devices. However, their practical application is hindered by low power density, material incompatibility, and electrode instability. In this study, a one-step synthesized gold nanoparticle-decorated graphene aerogel (GNP@GA) is developed as the negative electrode for GBFCs. The gold nanoparticles, exhibiting glucose oxidase-like catalytic activity, are firmly anchored onto the graphene aerogel framework. The aerogel structure provides a highly porous network that enhances ion transport, while the sp²-hybridized graphene ensures excellent electrical conductivity. The as-prepared GNP@GA electrode demonstrates a high current density and an extended voltage window. When paired with a platinum nanoparticle-deposited graphene aerogel (PNP@GA) positive electrode, the resulting GNP@GA//PNP@GA device achieves remarkable power and energy densities. Notably, the device maintains a high percentage of its initial current density over several days of continuous operation. These findings highlight a significant step toward the practical implementation of GBFCs for biomedical applications.

Keywords: Glucose biofuel cell, gold nanoparticles, Graphene aerogel, glucose-oxidase-like catalyst, stable electrode.

EFFICIENT AROMATIC C–H BOND OXYGENATION WITH OXOAMMONIUM SALT

Zeyu Wen^a, Yongtao Wang^{a, b, *}, Jia Yao^a, Haoran Li^{a, b, c, *},

^a Department of Chemistry, Zhejiang University, 866 Yuhangtang Rd, Hangzhou 310058, China

^b Center of Chemistry for Frontier Technologies, ZJU-NHU United R&D Center, Zhejiang University, 866 Yuhangtang Rd, Hangzhou 310058, China.

^c State Key Laboratory of Chemical Engineering, College of Chemical and Biological Engineering, Zhejiang University, 866 Yuhangtang Rd, Hangzhou 310058, China.

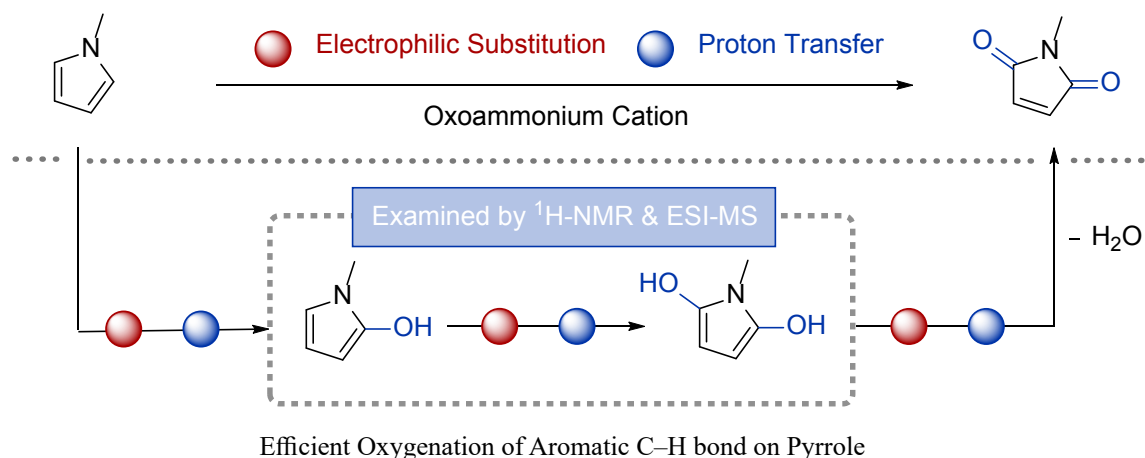
*Yongtao Wang: wyongtao@zju.edu.cn

*Haoran Li: lihr@zju.edu.cn

Abstract

Efficient selective oxygenation of aromatic C–H bonds have been challenging and attracting great interests from scientists and engineers. There have been sufficient researches on the efficiency enhancement and mechanism in-depth, involving radical pathways with dioxygen and aromatic electrophilic substitution (S_EAr) with hyperoxides. Following previous work of our group^{1,2}, an efficient S_EAr method for oxygenation of aromatic C–H bond on pyrrole ring will be reported in this work, where stoichiometric oxoammonium salts are used as oxidant. The reaction could reach full conversion within 1 minute and give yields of ~70% in selected solvent system. The substituent effect and solvent effect will be discussed as well as mechanism studies. As an exploration of the applications of oxoammonium salts, this work should give a new alternative for the oxygenation of aromatic C–H bonds.

Keywords: Aromatic C–H bonds, oxoammonium salts, oxygenation, S_EAr process, water.



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SUSTAINABLE TEXTILE CIRCULARITY: OPTIMIZING DYE REMOVAL FOR COTTON FIBER REGENERATION

Begoña González^{*,1}, Oscar Martínez-Rico¹, Ángeles Domínguez¹

¹Chemical Engineering Department, University of Vigo, Vigo, Spain

*Corresponding author: bgp@uvigo.es

Abstract

With the implementation of the EU Directive on waste (EU 2018/851) in 2025, the separate collection of textile waste has become mandatory, highlighting the urgent need for efficient recycling strategies. Currently, only 1% of textile fibers are derived from recycled materials, and the increasing demand for textiles continues to exacerbate environmental concerns [1]. The textile industry is a major contributor to global waste and pollution, with non-degradable waste textiles accumulating at an unsustainable rate. One of the key challenges in textile recycling is the removal of dyes from cotton fibers, as residual colorants can alter the properties of regenerated fabrics and hinder large-scale fiber reuse. Therefore, the development of an effective decolorization method is essential for advancing sustainable textile recycling.

In this study, a method for dye removal and fiber recycling was developed to facilitate the reintegration of cotton textiles into the production cycle. Aqueous N-methylmorpholine-N-oxide (NMMO) was utilized to achieve the separation of dyes from fibers while preserving fiber integrity. The process was found to efficiently extract dyes without significant degradation of the cotton structure, as confirmed by polymerization analysis. The recovered dyes were successfully isolated, with efficiencies dependent on dye structure. This approach represents a step toward industrial-scale textile recycling, providing a sustainable alternative for waste textile management and contributing to a circular economy in the textile sector.

Keywords: Textile sustainability, cotton, dye, NMMO

Acknowledgements

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SODIUM RICH LAYERED OXIDE CATHODES FOR HIGH CAPACITY SODIUM-ION BATTERIES

O. O. Thomas^{a,*}, R. A. House^b, P. G. Bruce^b,

^aDepartment of materials, University of Oxford, United Kingdom

*Corresponding author: oliver.thomas@materials.ox.ac.uk

Abstract

Recently there has been much interest in developing and understanding the chemistries of lithium-rich materials with stoichiometric ratios of $\text{Li:TM} > 1^{1-2}$ where TM is a transition metal. These materials can deliver improved capacity by redox involving the anions in the structure (i.e. $\text{O}^{2-} \rightarrow \text{O}^{(2-n)-} + n\text{e}^{-}$)³⁻⁵ to compensate Li^{+} removal. However, to meet the needs of a globally electrified society, electrochemical storage systems not reliant on lithium are required. Sodium-ion technologies are a promising alternative, but Na-ion batteries typically exhibit lower energy densities. Na-rich cathode technologies offer the opportunity to overcome this. However, the greater ionic radius of sodium means that for it to occupy a TM site, as Li^{+} does in Li-rich species, significant strain is induced. As such, most Na-rich species reported to date contain rare 2nd and 3rd-row transition metals Ru^{6,7} and Ir⁸, whose more diffuse orbitals can accommodate the larger Na^{+} ion. We have developed a synthetic approach which allows us to synthesise Na-rich materials using only earth abundant elements. These materials show great promise as the first industrially relevant Na-rich materials with the ability to undergo reversible (de)sodiation. Here our efforts to understand the charge compensation mechanism of these materials using various techniques including synchrotron spectroscopic (RIXS and XAS), and scattering (XRD and PDF) experiments are presented. From these studies we have resolved the charge compensation mechanism in these materials and demonstrated how it contrasts with that of Ru and Ir containing materials. This is critically valuable information for the rational design of energy materials as it reveals how we can control material behaviour through compositional tuning.

Keywords: Sustainable energy, Anionic redox, Spectroscopy, Diffraction, Energy materials

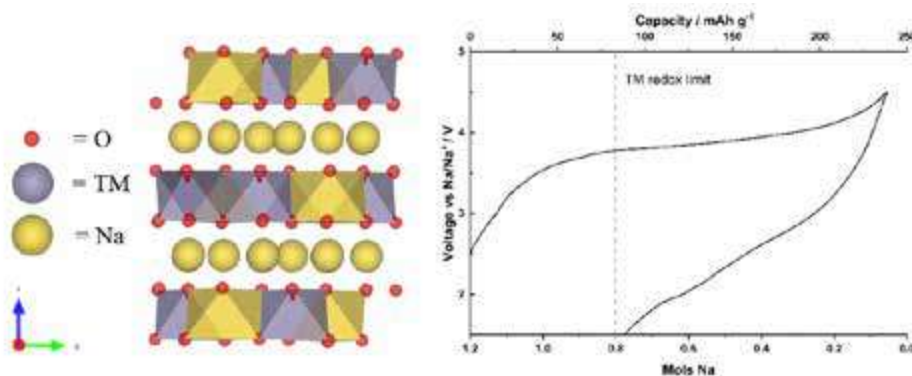


Figure 1: Left, structural model of a layered sodium (Na)-rich transition metal (TM) oxide. Right, First cycle charge-discharge curve of our novel material demonstrating the ability to remove almost all sodium from the structure with a charge capacity comparable to that of state of the art Li-ion materials

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SYNTHESIS OF ENVIRONMENTALLY FRIENDLY CATIONIC SURFACTANT FROM HEMP SEED OIL

Nergiz Cengiz^{a*}, İsmail Kasapoğlu^a,
^a*Tekirdağ Namık Kemal University, TÜRKİYE*
^{*}*Corresponding author: ncengiz@nku.edu.tr*

Abstract

Traditional fabric softeners are water-based structures containing 10-15% double-tailed dialkyldimethyl ammonium surfactants and, mainly produced from palm oil. Since these structures are not biodegradable, they have been developed recently by replacing the dialkyldimethylammonium moieties with cationic surfactants called esterquats. However, the fact that most of the synthesized esterquat structures are derived from palm oil is of concern. The overproduction and the magnitude of the environmental costs of palm oil are the subjects of intense criticism. Significant risks include the destruction of natural forests to plant palm trees, the reduction of biodiversity, and damage to the ecosystem by affecting clean air, soil, water, and nutrient cycles. Therefore, there is a need for textile softeners that are naturally sourced, environmentally friendly, easily accessible, and inexpensive.

As far as we know, the hemp plant requires less water, fewer pesticides and fertilizers, is easy to grow anywhere in the world, and at the same time has high oxygen production, and has not been investigated as a raw material for fabric softener in the textile field. This research aims to synthesize an esterquat-based cationic surfactant using hemp seed oil to and to investigate its softening properties.

Keywords: esterquat-based cationic surfactant, hemp seed oil, fabric softener, environmentally friendly

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GREEN SYNTHESIS OF COPPER (II) OXIDE NANOPARTICLES (CuO-NPs) BY USING A MIXTURE OF FERMENTED RABBIT URINE AND GOLDEN APPLE SNAIL AS REDUCING AGENT

Saiyidah Nafisah Hashim^a, Nurul Izza Taib^{a,*},

^a*Faculty of Applied Sciences, Universiti Teknologi MARA, Perak Branch, Tapah Campus, 35400 Tapah Road, Perak, Malaysia.*

^{*}*Corresponding author: izza257@uitm.edu.my*

Abstract

In this study, CuO nanoparticles were successfully synthesized using fermented rabbit urine and golden apple snail (RUG) as reducing agents. The biosynthesis process was conducted at 50 °C, where copper (II) sulfate solution was mixed with the prepared bio-reducing mixture, leading to the immediate formation of CuO nanoparticles, confirmed by the characteristic colour change. The synthesized nanoparticles were characterized using UV-Vis spectroscopy, Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX). The results revealed the formation of predominantly irregular-shaped CuO nanoparticles with average sizes ranging from 30–50 nm, displaying good crystallinity and purity. FTIR analysis indicated the presence of bioactive compounds responsible for reduction and stabilization, while XRD confirmed the monoclinic phase of CuO¹. The significance of this study lies in its rapid, low-cost, and green synthesis strategy, providing an accessible approach for nanoparticle production using locally available biological resources. Furthermore, the synergistic effect of fermented rabbit urine and golden apple snail extract enhances the reducing capacity and stability of the synthesized CuO NPs, making this method highly promising for applications in environmental remediation, catalysis, and biomedical fields.

Keywords: green synthesis, CuO nanoparticles, rabbit urine, golden apple snails, reducing agents

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ENHANCED HYDROGEN PRODUCTION VIA FORMIC ACID DEHYDROGENATION USING TRIMETALLIC PDNICO NANOPARTICLES ENCAPSULATED IN MOFS

Noor Hayati Ridhwan^a, Najihah Syahbudin^a, Muhammad Shafie Norhisham^a, Norliza Dzakaria^{a,b,*},
Nurul Auni Zainal Abidin^a, Azizul Hakim^c, Arrozi, U. S. F^d

^a*School of Applied Science and Environment, Faculty of Applied Science,
Universiti Teknologi MARA(UiTM), Cawangan Negeri Sembilan, Kampus Kuala Pilah,
72000 Kuala Pilah, Negeri Sembilan, Malaysia.*

^b*Advanced Material for Environmental Remediation (AMER),
Universiti Teknologi MARA(UiTM), Cawangan Negeri Sembilan, Kampus Kuala Pilah,
72000 Kuala Pilah, Negeri Sembilan, Malaysia*

^c*Department of Science and Technology, Universiti Putra Malaysia Bintulu Campus, Nyabau Road, P.O Box 396,
97008 Bintulu, Sarawak, Malaysia*

^d*Department of Chemistry, Universitas Negeri Malang Jl. Semarang No. 5, Malang*

*Corresponding author: norliza864@uitm.edu.my

Abstract

This study investigates trimetallic PdNiCo nanoparticles encapsulated within NH₂-BDC and UiO-66-NH₂-BDC Metal-Organic Frameworks (MOFs) for efficient hydrogen production via formic acid dehydrogenation. Catalysts were synthesized using solvothermal methods, yielding PdNiCo-NH₂ BDC, which exhibited partial crystallinity, and PdNiCo-UiO-66-NH₂-BDC, characterized by high crystallinity. XRD analysis confirmed structural differences, where the crystalline structure of UiO-66-NH₂ BDC enhances charge transfer efficiency and framework stability, unlike NH₂-BDC. FTIR-ATR identified a distinct Zr-O vibration at 690 cm⁻¹ in UiO-66-NH₂-BDC, stabilizing metal-MOF interactions and optimizing reaction pathways. BET analysis showed a significantly higher surface area for PdNiCo-UiO-66-NH₂-BDC (459.8 m²/g) compared to PdNiCo-NH₂-BDC (14.7 m²/g). Morphological studies using FESEM and TEM showed more uniform and well-dispersed nanoparticles in the crystalline UiO-66-NH₂ framework. TEM analysis showed smaller, more dispersed nanoparticles (220 nm) in PdNiCo-UiO-66-NH₂-BDC versus agglomerated structures (600 nm) in PdNiCo-NH₂-BDC. Catalytic testing demonstrated PdNiCo-UiO-66-NH₂-BDC's superior performance, achieving 98% H₂ selectivity and 92% conversion efficiency at 80°C with 0.5 M formic acid, outperforming PdNiCo-NH₂-BDC (74% conversion). The enhanced activity correlates with the crystallinity of UiO-66-NH₂-BDC, its higher surface area, and optimized active-site accessibility. These results highlight PdNiCo-UiO-66-NH₂-BDC as a scalable, stable catalyst for sustainable hydrogen production, with performance tunable via temperature and concentration adjustments.

Keywords: Metal Organic Frameworks, UiO-66-NH₂-BDC, NH₂-BDC, trimetallic, formic acid, dehydrogenation

ION-EXCHANGE MEDIATED PHOTOCHEMICAL PRODUCTION OF ULTRAHIGH LOADING SINGLE-ATOM CATALYSTS

Huang Yucong^a, Chen Zhongxin^{a,*}

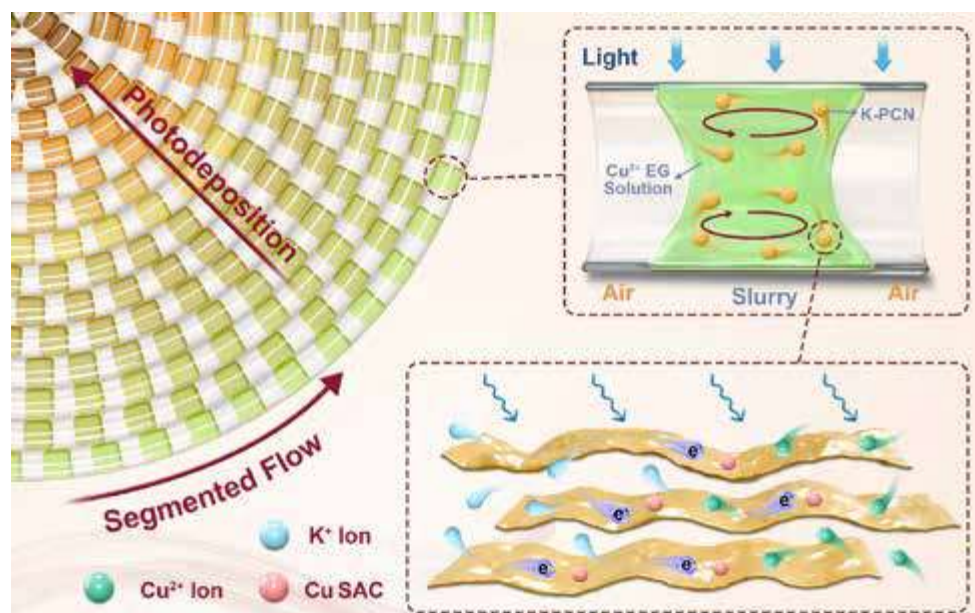
^aThe Chinese University of Hong Kong, Shenzhen

*Corresponding author: chenzhongxin@cuhk.edu.cn

Abstract

Single-atom catalysts (SACs) represent a revolutionary advancement in catalysis, offering exceptional atom efficiency by dispersing isolated metal atoms on a support material. However, achieving high metal loading (>10 wt.%)—crucial for enhancing catalytic activity and enabling synergistic effects in complex reactions—has traditionally relied on energy-intensive pyrolysis, while milder photosynthetic methods struggle to exceed 5 wt.%². This study introduces a potassium pre-installation strategy that overcomes the thermodynamic and kinetic barriers of photosynthetic SAC synthesis. By integrating potassium ions into polymeric carbon nitride (PCN), we enable ion exchange-driven anchoring of metal atoms, bypassing the need for high-temperature bond activation. Coupled with a slurry continuous-flow photosynthesis process, this approach yields an ultra-high loading Cu₁/PCN catalyst (>18 wt.%) with atomic dispersion, confirmed through extensive characterization. The catalyst excels in C-O coupling reactions, achieving high yields under ligand-free conditions. Compared to pyrolysis, this method offers lower energy use, scalability, and cost-effectiveness, as validated by techno-economic analysis, paving the way for sustainable, large-scale high loading SAC production.

Keywords: Continuous-Flow Production • Segmented Flow • Photodeposition • Single Atom Catalysts



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SOLID-PHASE UPCYCLING TOWARD THE PRODUCTION OF ULTRAHIGH-LOADING SINGLE-ATOM CATALYSTS

Guanwu Lian^{1#}, Zefan Du^{1#}, Yifan Wang^{1#}, Yelan Xiao^{2,*}, Mengyao Su³, Chao Wu⁴, Yucong Huang¹, Yuansheng Lin¹, Jingjing Xiong¹, Yichen Chen¹, Shibo Xi⁴, Wenguang Tu¹, Zhigang Zou^{1,*}, Zhongxin Chen^{1,*}

¹ School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, Guangdong, 518172, China.

² Shenzhen Key Laboratory of Nano-Biosensing Technology, Marshall Laboratory of Biomedical Engineering, School of Biomedical Engineering, Shenzhen University Medical School, Shenzhen University, Shenzhen 518060, China.

³ Department of Applied Physics, Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China.

⁴ Institute of Chemical and Engineering Sciences, Agency for Science, Technology and Research (A*STAR), 1 Pesek Road, Jurong Island, Singapore 627833, Singapore.

*Corresponding author: chenzhongxin@cuhk.edu.cn

Abstract

The recovery of valuable transition metals from deactivated catalysts is crucial for alleviating the challenges of resource scarcity and environmental pollution. Guided by AI-powered big data analysis, we identified an important research gap in the sustainable recovery of early transition metals and proposed a solid-phase upcycling strategy to transform waste catalysts into highly valuable single-atom catalysts (SACs). This involves a heat-induced redispersion of metal aggregates into single atoms on the polycrystalline carbon nitride (PCN) support, producing highly active M₁-PCN SACs up to 20 wt% (M = Cu, Fe, Co, and Ni). Subsequent techno-economic analysis confirms a two-third reduction in production cost and greenhouse gas emissions compared to conventional hydrometallurgical and pyrometallurgical processes, thus paving a new path in the development of sustainable technologies for metal recovery.

Keywords: Solid-phase upcycling, single-atom catalysts, big-data analysis, techno-economic analysis, dynamic aggregation.



Figure 1. Solid-phase upcycling process of ultrahigh loading SACs

AN ALTERNATIVE APPROACH TO THE PLANT PROTECTION WITH THE USE OF NOVEL IONIC DERIVATIVES OF SALICYLIC ACID AND BENZOTHIADIAZOLE

Maciej Spychalski^{a,b,*}, Rafal Kukawka^{a,b}, Artur Strzeliński^c, Zuzanna Sawinska^d, Agnieszka Kiniec^e,
Renata Gaj^f, Marcin Smiglak^a,

^a Poznan Science and Technology Park, Adam Mickiewicz University Foundation,
ul. Rubiez 46, 61-612 Poznan, Poland.

^b ATI Sp. z o.o., ul. Rubiez 46, 61-612 Poznan, Poland

^c Experimental Farm Zlotniki, Poznań University of Life Sciences, Poznan, Poland;

^d Department of Agronomy, Poznań University of Life Sciences, Poznan, Poland;

^e Regional Experimental Station in Torun, Institute of Plant Protection - National Research Institute, Torun,
Poland;

^f Department of Agricultural Chemistry and Environmental Biogeochemistry, Poznan University of Life Sciences,
Poznan, Poland;

*Corresponding author: maciej.spychalski@ppnt.poznan.pl

Abstract

The urgent need for sustainable development, recommended by the European Union and expressed in the “Farm to Fork Strategy”, includes a serious restriction on the use of plant protection products (PPPs). This strategy assumes a 50% reduction in the use of PPPs by 2030. These efforts have driven the exploration of innovative and effective plant protection strategies utilizing new active compounds that can serve as an alternative to PPPs.¹

The phenomenon of SAR (systemic acquired resistance) constitutes one of the defence mechanisms of plants against pathogens. The plant's response understood as the stimulation of its acquired resistance may be activated in response to the action of the pathogen, but also in response to the action of an elicitor. The SAR inducers, whose activity has been extensively studied are benzo(1.2.3)thiadiazole-7-carboxylic acid, S-methyl ester and salicylic acid. We used the concept of ionic liquids to modify these compounds in order to improve their physicochemical properties and biological activity.²

The general aim of this study undertaken was to check the effect of using novel active substances, being an ionic derivatives of salicylic acid and benzothiadiazole³ on the field cultivation of winter wheat and potatoes. The tested treatment variants include variants where only novel SAR inducers were applied as well as variants of combined use of SAR inducers and fungicides.

The results indicate that the use of the tested active substances may be an alternative to PPPs in the context of providing effective protection against diseases. Moreover, a significant increase in quantitative and qualitative parameters was observed in comparison to the untreated control variant.

This research was supported by The National Centre for Research and Development (Poland), project LIDER (LIDER13/0211/2022) - “Growth and development stimulants with immunity-inducing effect as an innovative product for use in the cultivation of agricultural consumer plants”.

Keywords: ionic liquid, systemic resistance inducers, salicylic acid, benzothiadiazole, winter wheat, potato

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AMORPHOUS-CRYSTALLINE INTERFACE INDUCED INTERNAL ELECTRIC FIELDS FOR ELECTROCHROMIC SMART WINDOW

Shi Zhang^a, Xun Hong^{a,*}

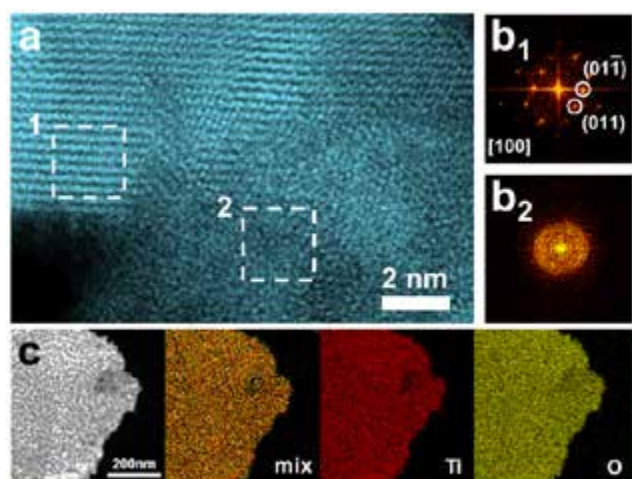
^aUniversity of Science and Technology of China

*Corresponding author: hongxun@ustc.edu.cn

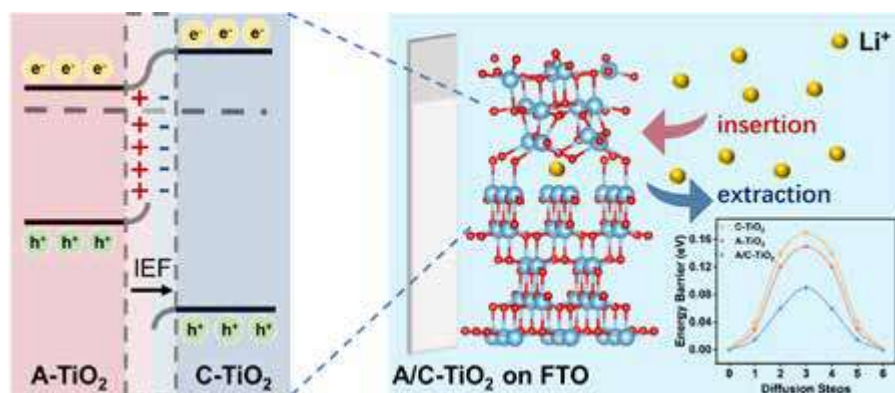
Abstract

Balancing optical modulation and response time is crucial for achieving high coloration efficiency in electrochromic materials. Here, internal electric fields are introduced to titanium dioxide nanosheets by constructing abundant amorphous-crystalline interfaces, ensuring large optical modulation while reducing response time and therefore improving coloration efficiency. Aberration-corrected high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) reveals the presence of numerous amorphous-crystalline phase boundaries in titanium dioxide nanosheets. Kelvin probe force microscopy (KPFM) exhibits an intense surface potential distribution, demonstrating the presence of internal electric fields (IEF). Density functional theory (DFT) calculations confirm that the amorphous-crystalline heterointerfaces can generate internal electric fields and reduce diffusion barriers of lithium ions. As a result, the amorphous-crystalline titanium dioxide nanosheets (A/C-TiO₂) exhibit better coloration efficiency (35.1 cm² C⁻¹) than pure amorphous (A-TiO₂) and crystalline (C-TiO₂) titanium dioxide nanosheets.

Keywords: amorphous-crystalline, electrochromic, smart window, TiO₂



1. Titanium dioxide nanosheets with abundant amorphous - crystalline heterogeneous interfaces



2. The IEF at the heterogeneous interface is conducive to reducing the diffusion energy barrier of Li⁺

NUCLEOPHILIC ACTIVATION OF ELEMENTAL CHALCOGENES IN THE PRESENCE OF IONIC LIQUIDS

Natalia Tarasova^{a,*}, Efrem Krivoborodov^a,
Samson Muradyan^a, Darya Andriyanova^a

^aDmitry Mendeleev University of Chemical Technology of Russia

*Corresponding author: tarasova.n.p@mucrt.ru

Abstract

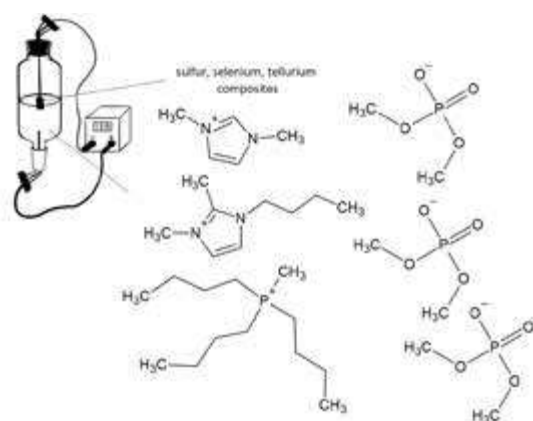
For many decades now, chalcogen-based materials have been intensively studied with respect to various applications, e.g. as basic components for energy storage. In this context, metal-sulfur batteries stand out due to their high energy density, specific capacity and relatively low cost. Metal tellurides play an important role as thermoelectrics, topological insulators, ionic conductors and materials with high magnetoresistance. Selenium is widely used for X-ray and γ -ray detectors as well as in solar cells because it offers high photoconductivity, high absorption coefficient and can be easily deposited as layers even on large surfaces [1].

Reaction processes involving elemental chalcogenes require energy costs, since at the first stage of any chemical process it is necessary to convert elemental chalcogenes into a reactive form. In this connection, research work on reducing energy costs for the activation of elemental sulfur, selenium, and tellurium by means of ionic liquids is already underway at the D. Mendeleev University of Chemical Technology of Russia.

Ionic liquids have a number of advantages over traditional organic reagents in the context of compliance with the principles of green chemistry in the implementation of chemical interactions, as they are non-flammable, non-volatile compounds and do not pose a threat to the environment.

The localization of negative charge in anions of some ionic liquids promotes the initiation of nucleophilic interaction of these ionic liquids with chalcogenes already at room temperature [2]. To intensify this process, we proposed to use an electrochemical cell where the anode is any metallic element, for example, platinum, and the cathode is pure chalcogen or carbon chalcogen-containing material. At maintaining a voltage of 1.5 V, the transfer of chalcogen into the active form stabilized by the ionic liquid medium is fixed, which opens the way to the use of this technique in order to obtain chalcogen-containing materials, coatings or new compounds.

Keywords: elemental sulfur; elemental selenium; elemental tellurium; ionic liquids; chalcogenes; green chemistry.



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ADVANCING GREEN CHEMISTRY THROUGH THE ECO-FRIENDLY SYNTHESIS AND APPLICATIONS OF FUNCTIONAL MATERIALS

Aurelia Vișă^{a,*}, Marcela Iosivoni^a, Nicoleta Pleșu^a, Bianca Maranescu^b

^aRomanian Academy, "Coriolan Drăgulescu" Institute of Chemistry, 24 Mihai Viteazu Blv, 300223 Timișoara, România, *Corresponding author: apascariu@yahoo.com

^bDepartment of Biology-Chemistry, Faculty of Chemistry, Biology, Geography, West University, 16 Pestalozzi Street, 300115 Timisoara, Romania

Abstract

Functional materials encompass various material classes designed for specific applications by tailoring their properties. Metal-Organic Frameworks (MOFs) are a class of functional materials, recognized by their exceptional adaptability with applications in sensing, gas storage, catalysis, drug delivery, and environmental remediation. Green approaches to MOF synthesis aim to reduce environmental effects by lowering hazardous chemicals, waste creation, and energy usage, all while maintaining or improving the materials characteristics and performance^{1,2}.

In this perspective, it is herein reported our recent work on some illustrative examples of how MOFs can be synthesized using greener alternative reaction pathways, Figure 1, such as solvent-free mechanochemical synthesis, microwave, ultrasound-assisted techniques, electrochemical, and the use of eco-friendly solvents.

Several two-component or three-component MOFs synthesis and their applications in catalysis, as adsorbent materials for water pollution remediation, or their electrochemical activity of metal phosphides are presented, starting from various *metals*: Co, Ni, Zn, Cu; *Ce*, *phosphonic acids*: vinylphosphonic acid, phosphonoacetic acid, 1-hydroxyethylidene-1,1-diphosphonic acid; and *co-ligand* imidazole (Im)^{3,4}. This knowledge will present new opportunities and challenges for future research⁵.

Keywords: green chemistry, metal organic frameworks, phosphonates

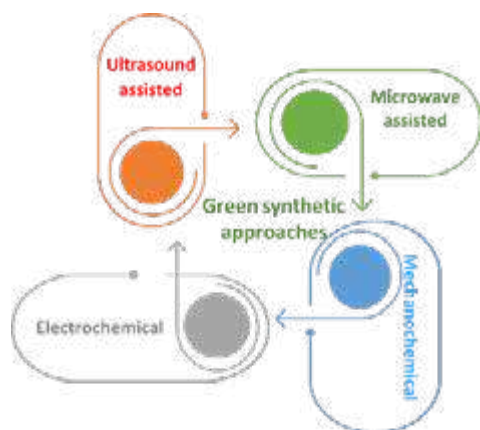


Figure 1. Eco-friendly synthesis of functional materials

Acknowledgements:

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CATALYSIS AND SUSTAINABILITY FROM ATOM TO PLANETARY SCALE

Javier Pérez-Ramírez

Institute for Chemical and Bioengineering and NCCR Catalysis, ETH Zurich, Switzerland

**Corresponding author: jpr@chem.ethz.ch*

Abstract

Ensuring a sustainable future for the chemicals and energy industries is a pressing global concern that has far-reaching impacts on the environment, human health, quality of life, and the economy. Catalysis plays a crucial role in this journey, constantly pushing the boundaries of conventional design to spearhead the transition towards defossilized and circular chemical manufacturing. This talk aims to illustrate the interdisciplinary and cross-scale mindset required to design catalysts that meet the ever-evolving sustainability criteria, bridging the gap between atom and planet.¹ Delving into the latest research from my laboratory, I will showcase how a deeper understanding of catalyzed processes is driving revolutionary technological advancements. Through case studies in key areas such as CO₂ valorization, polymer manufacture, and organic synthesis, I will exemplify how nanoscale engineering and the availability of increasingly powerful tools to access structural variations and mechanism under relevant conditions aid catalyst discovery. At the forefront of design, I will demonstrate the importance of precisely controlling the architecture, speciation, and dynamics of supported metals in low-nuclearity catalysts, highlighting the impact that even the smallest changes can have on performance. The presentation will touch on current frontiers in catalyst synthesis and characterization, and emphasize the critical role of quantitative metrics in guiding low-carbon strategies.

Keywords: Catalysis, Nanoscale engineering, Circular carbon, Green chemistry, Sustainability

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GREEN APPROACHES TO RECYCLING OF POLYESTER WASTES INTO CHEMICALS

Zhimin Liu*

^aInstitute of Chemistry, Chinese Academy of Sciences

**Corresponding author: liuzm@iccas.ac.cn*

Abstract

Chemical recycling of plastics into monomers or value-added chemicals is one of pivotal accesses to achieve a circular economy in the plastic life cycle, which also provides important way to access chemicals. Polyesters are a kind of major plastics widely applied in our life, and the spent polyesters can be decomposed via various strategies such as hydrolysis, alcoholysis, hydrogenolysis, aminolysis, which has attracted much attention. In our recent work, we developed several simple, green and highly efficient routes to depolymerize polyesters into their monomers and/or valuable chemicals, and the catalytic mechanism was also investigated.¹⁻⁶ For example, we presented ionic liquid-catalyzed aminolysis of polyesters including poly(lactic acid),¹ poly(bisphenol A carbonate)¹ and poly(succinates)², and a series of N-containing chemicals such as N-aryl lactamides, ureas and N-substituted succinimides were accessed in high yields. We reported a novel and general strategy to degrade polyesters via directly breaking the C_{alkoxy}-O bond by nucleophilic substitution of halide anion of ionic liquids under mild conditions, producing relevant unsaturated carboxylic acids and alkenes, and in the presence of hydrogen and Pd/C saturated carboxylic acids and alkanes were obtained.³ We designed different catalytic systems for polyester degradation. Anatase TiO₂ supported Ru and Mo dual-atom catalysts achieved transformation of various polyesters into corresponding diols in 100% selectivity via hydrolysis and subsequent hydrogenation in water under mild conditions,⁴ and the ionic liquid-Pt/TiO₂ catalytic system achieved oxidative degradation of polycaprolactone with air into adipic acid via hydrolysis and subsequent oxidation in water.⁵ We also reported a novel strategy to upcycle polyamide wastes to tertiary amines with the assistance of H₂ in acetic acid under mild conditions, which was achieved over anatase TiO₂ supported Mo single atoms and Rh nanoparticles.⁶ I will present our recent work at the Symposium.

Keywords: Polyester wastes, recycling, chemicals, ionic liquids, catalyst

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DIRECT AND INDIRECT HOTSPOTS AS PRIORITIES FOR GREEN CHEMISTRY RESEARCH

Philip G. Jessop^{a,*} and Alex R. MacDonald^a

^a*Department of Chemistry, Queen's University, Kingston, ON, Canada, K7L 3N6.*

^{*}*Corresponding author: jessop@queensu.ca*

Abstract

Green chemistry researchers are motivated to use our research to benefit the environment, reduce harm, and help society become more sustainable. However, not all research projects are equally helpful to the environment. We should prioritize projects that should maximize the benefit. When undertaking research aimed at reducing the harm of a multistep process or life cycle greener, The concepts of *direct and indirect hotspots* can help us prioritize. One obvious strategy is to focus on making the most harmful steps (the direct hotspots) greener. That's much more effective than spending time greening a part of the process that isn't a hotspot.¹ While that strategy may seem obvious, it hasn't been much practiced in green chemistry research because life cycle assessment (LCA) data for pinpointing hotspots has been largely unavailable. Now that LCA data is becoming more commonplace, this strategy should take on greater importance.

However, counter-intuitively, it is sometimes more effective to modify a step that is NOT a hotspot – and not by making it greener. Certain steps are indirect hotspots, meaning they cause little harm but they have an outsized influence on the total harm of a process. It may, quite often, be better for the environment if we make such a step more harmful! In some situations, such a modification of an indirect hotspot will greatly reduce the harm of the direct hotspot and, thereby, the harm of the entire process.²

This presentation will explain direct and indirect hotspots, and describe how research chemists and chemical engineers can use these concepts to prioritize efforts to reduce the harm of multistep processes. Examples will be given from the author's research into CO₂-switchable technologies for greener coatings and adhesives.

Keywords: green chemistry, life cycle assessment, chemical synthesis, polymers, coatings

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TOWARD GREEN SYNTHETIC APPROACHES OF C6 BIO-BASED PLATFORM CHEMICALS

Fabio Aricò

*^aDepartment of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Via Torino
155, 30170 Venezia Mestre (IT)*

**Corresponding author: Fabio.arico@unive.it*

Abstract

The integration of basic sciences into sustainable development is a key focus for many global initiatives, including the International Year of Basic Sciences for Sustainable Development and the United Nations Agenda 2030, which highlights 17 Sustainable Development Goals (SDGs). Organic synthesis plays a crucial role in addressing sustainability challenges such as using non-harmful reagents, minimizing energy and waste, and promoting recycling. These principles are central to the efforts of numerous international organizations, including the International Union of Pure and Applied Chemistry (IUPAC).

The discovery, development, and application of new organic synthesis methods, along with an understanding of their reaction mechanisms, is an essential area of research. In this context, dialkyl carbonates (DACs) have gained significant attention over recent decades due to their benign nature.¹ Dimethyl carbonate (DMC), in particular, has become a vital substitute for chlorine-based chemicals in various chemical reactions. While halogen-based molecules are more reactive, they often lack selectivity in chemical reactions. In contrast, DACs tend to offer high selectivity in alkylation reactions despite their lower reactivity. Green syntheses using DMC have been reported in the production of anti-inflammatory drugs, polymers, fragrances, and solvents. DACs are also utilized as fuel additives, lithium battery solvents, and in the manufacture of pharmaceuticals, pesticides, plastics, coatings, electronics, and agrochemicals.

This lecture focuses on the use of DMC and other DACs as alternatives to halogen-based compounds in the synthesis and derivatization of bio-based platform chemicals such as isosorbide, galactaric acid and furanic compounds derived from D-Fructose.² Assessments of the greenness of the abovementioned procedures were evaluated via Green metrics.

Keywords: Bio-based platform chemicals, , Isosorbide, Galactaric acid, HMF, Green Metrics

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SEQUESTRATION OF ENVIRONMENTAL CONTAMINANTS USING POROUS HYBRID NANOADSORBENTS: A STEP TOWARDS SUSTAINABLE ENVIRONMENT

Sahel Fajal^a, and Sujit K. Ghosh^{a,b,*}

^aDepartment of Chemistry, Indian Institute of Science Education and Research (IISER) Pune, Dr Homi Bhabha Road, Pashan, Pune 411008, India.

^bCentre for Water Research (CWR), Indian Institute of Science Education and Research (IISER) Pune, Dr Homi Bhabha Road, Pashan, Pune 411008, India.

*Corresponding author: sghosh@iiserpune.ac.in

Abstract

Environmental remediation using porous materials is a promising approach in green chemistry, as these materials can effectively absorb and remove pollutants from water and air. Their high surface area and tunable porosity enable selective binding of contaminants, such as heavy metals and organic compounds, while minimizing the use of hazardous chemicals. Innovations in this field include the development of bio-inspired and sustainable porous materials, such as metal-organic frameworks (MOFs), covalent-organic frameworks (COFs), which not only enhance pollutant capture but also promote regeneration and reuse. By integrating these materials into remediation strategies, we can achieve a more sustainable and efficient cleanup of contaminated environments, aligning with the principles of green chemistry.^{1,2} In the pursuit of mitigating environmental challenges such as pollution, climate change, and resource depletion, the development of advanced functional porous materials has emerged as a promising avenue for innovative solutions. These porous materials are garnering increasing attention for their ability to sequester and efficiently separate various toxic substances from the surroundings. From greenhouse gas capture to the removal of hazardous pollutants from air and water, advanced functional porous materials have demonstrated remarkable versatility and effectiveness in addressing pressing global issues. The developed materials are employed as a method for the sequestration application of toxic guest species that are environmentally hazardous. On the basis of the principles of ion exchange and host-guest interactions, efforts have been made to design functional porous frameworks and their hybrid composites for the effective separation of various environmentally toxic gases (radioactive organic iodides and iodine species) and water contaminants (organic pollutants and inorganic metal-oxoanionic species).³⁻⁶

Keywords: Environmental remediation, Chemical separation, Sustainable environment, Water purification, Toxic gas capture, Porous materials, MOFs, COFs

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THE GLOBAL CONVERSATION ON SUSTAINABILITY: AN IUPAC/IYCN JOINT EFFORT TOWARDS A MORE SUSTAINABLE FUTURE THROUGH CHEMISTRY

João Borges^{a,*}, Juliana L. Vidal^b

^aCICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

^bBeyond Benign, 18 Church Street, 1016, Wilmington, MA, USA

*Corresponding author: joaoborges@ua.pt

Abstract

The development of strategies for raising awareness, communicating, collaborating, and taking action to impart a culture of sustainable practices in scientists and society through chemistry is vital for addressing the United Nations Sustainable Development Goals (UN SDGs). In this regard, the fields of green and sustainable chemistry provide a holistic framework capable of interconnecting several aspects of our society, thus providing scientists and citizens with the tools to assess, design, and implement benign approaches and strategies for achieving a sustainable future.

In this talk, we will introduce the ‘Global Conversation on Sustainability (GCS)’ [1], a joint project led by the International Union of Pure and Applied Chemistry (IUPAC) and the International Younger Chemists Network (IYCN), and supported by the IUPAC Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD) – project no. 2021-034-2-041. The GCS project aims to bring the global chemistry community together and foster a multi-stakeholder dialogue in discussing activities and actions pursued locally, nationally and internationally, as well as collaborative efforts for effectively communicating and actively implementing a culture of green and sustainable chemistry practices across multiple audiences to address the UN SDGs. We will introduce the goals, strategies and initiatives put forward by the GCS project, including GCS Day, articles in peer-reviewed journals [2] and science news magazines [3], special issues [4], and symposia in international conferences aiming to raise awareness, inspire and meaningfully engage the chemistry community and society in the discussion to promote the UN SDGs. The GCS is a global and inclusive platform, aligned with the goals and mission of both IUPAC and the IYCN, to promote change. In this presentation, we aim to inspire, encourage, and empower scientists and citizens to actively join us in contributing to this global effort towards a safer, healthier and ‘greener’ world.

Keywords: UN SDGs, sustainability, education, collaboration, society



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IN SITU ENCAPSULATION OF CATIONIC [2]CATENANE IN A STABLE ZIRCONIUM METAL-ORGANIC FRAMEWORK IN WATER

Shuliang Yang^{a,*}, Yang Jiao^{b,*}, J. Fraser Stoddart^{c,*}

^aCollege of Energy, Xiamen University, Xiamen, 361005, Fujian, China

^bCollege of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

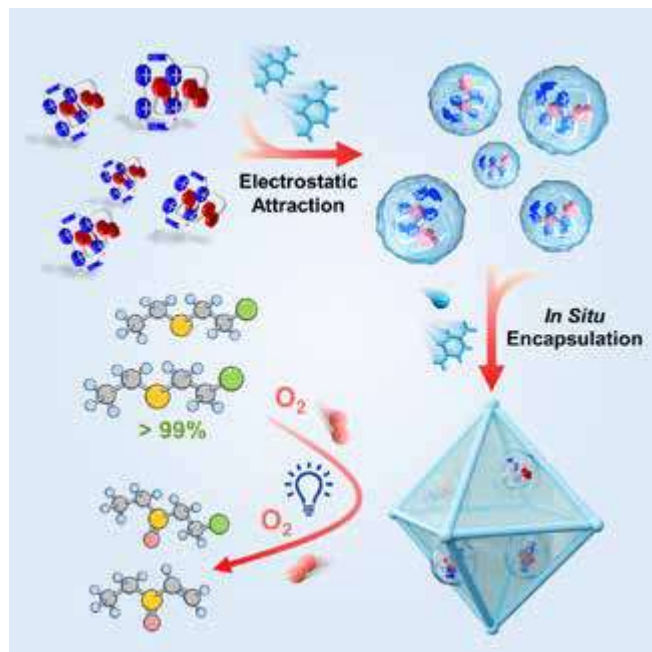
^cDepartment of Chemistry, Northwestern University, Evanston, Illinois 60208, United States

*Corresponding author: ysl@xmu.edu.cn, jiaoyang2023@pku.edu.cn, stoddart@northwestern.edu

Abstract

As an emerged class of porous support, metal-organic frameworks can host multifarious guests to realize diverse applications. Among the guest-introducing approaches, *in situ* encapsulation method is unique in its ability to incorporate a diverse range of guests, from small organic molecules, metal clusters to proteins and even more complicated guests. Previous investigations have focused on guests that are either neutral or negatively charged. The realization of *in situ* encapsulation of cationic catenanes in metal-organic frameworks under mild conditions, however, has rarely been investigated. Herein, we have accomplished *in situ* encapsulation of a cationic catenane (DA[2]C) within UiO-66-F₄—a metal-organic framework consisting of Zr₆ nodes and tetrafluoroterephthalic acid ligands—at room temperature using H₂O as a green solvent. Theoretical calculations elaborated that tetrafluoroterephthalic acid ligands interact strongly with the cationic DA[2]C. This observation is a result of electrostatic interactions between carboxylate anions and DA[2]C cations, as well as the attraction of electronegative F atoms in tetrafluoroterephthalic acid to the cations. As a proof-of-concept application, DA[2]C•4Cl/UiO-66-F₄ composite demonstrated heterogeneous catalytic detoxification of 2-chloroethyl ethyl sulfide to the sulfoxide with complete conversion rate (> 99%) and high selectivity (> 97%). This method could also be extended to other organic cationic molecules including dibenzyl benzoimidazoloimidazole chloride and a pyrene-functionalized cyclobis(paraquat-*p*-phenylene), rendering it as a universal platform for constructing host-guest MOF systems with various applications.

Keywords: mechanically interlocked molecules, catenanes, cationic guests, in situ encapsulation, metal-organic framework



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FROM GREEN CHEMISTRY TO CLEAN WATER: SYNTHESIS AND APPLICATIONS OF STABLE COVALENT ORGANIC FRAMEWORKS

Li Peng

College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian, 361005, China

*Corresponding author: li.peng@xmu.edu.cn

Abstract

The quality of covalent organic frameworks (COFs) is vital for their applications, yet structural damage during activation remains a major challenge. This presentation introduces two innovative strategies to synthesize high-quality COFs with enhanced stability and functionality. The first strategy utilizes functional polymer guests, such as polydopamine (PDA), to stabilize COF structures. Polymers act as supportive pillars, preventing pore collapse and maintaining high porosity and crystallinity. For instance, the TAPB-TA/PDA composite achieves a 16-fold increase in surface area compared to its parent COF. The reinforced structure also enhances photocatalytic hydrogen evolution by improving charge carrier transport. Molecular dynamics simulations confirm that PDA oligomers reinforce COF walls through van der Waals interactions, preserving structural integrity. The second approach employs a self-sacrificing guest method, where salt guests are incorporated into COF pores to provide structural support during activation. Upon heating, the salts decompose into gases, yielding highly pure COFs without residual guests. This method produces twelve SG-COFs with superior crystallinity and porosity, demonstrating exceptional performance as adsorbents for per- and polyfluoroalkyl substances (PFAS). Together, these approaches- polymer stabilization and self-sacrificing salts-address key challenges in COF synthesis, enabling high-quality frameworks with expanded applications in environmental remediation, catalysis, and beyond.

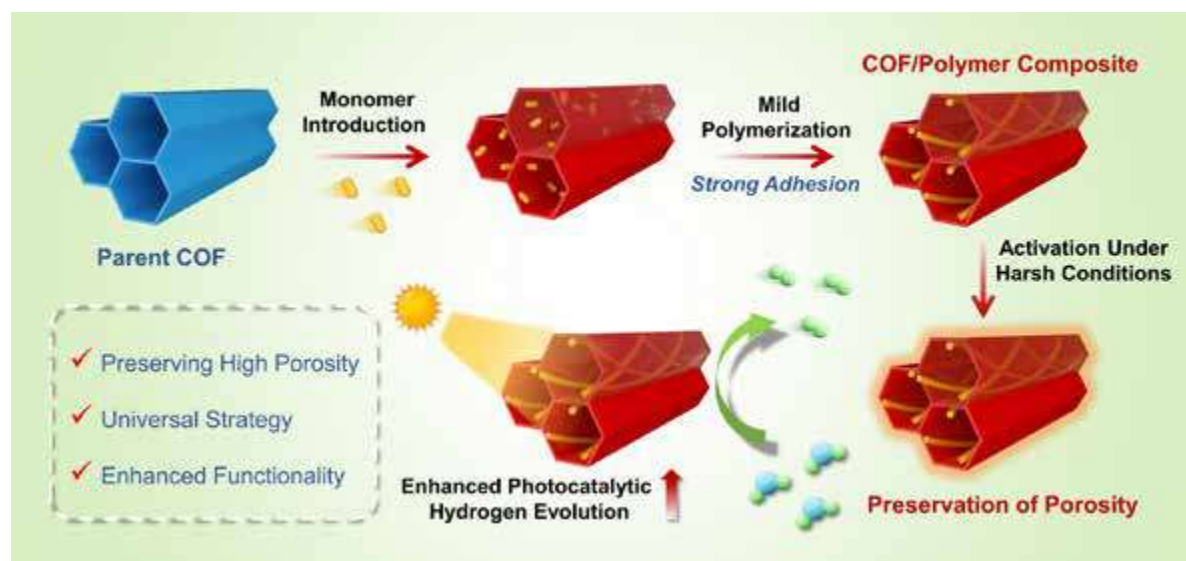


Figure 1 Schematic illustration for COF synthesized through polymer introduction.

Keywords: Covalent Organic Frameworks, Self-Sacrificing Guest Method, Polymer Stabilization, Structural Integrity, Environmental Remediation

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FORMIC ACID-ASSISTED DEOXYGENATION OF FATTY ACIDS INTO GREEN DIESEL, FATTY-KETONES AND -ALDEHYDES

Banothile C.E. Makhubela^{a*}, Sibongle Pikoli^a, Avela Kunene^a

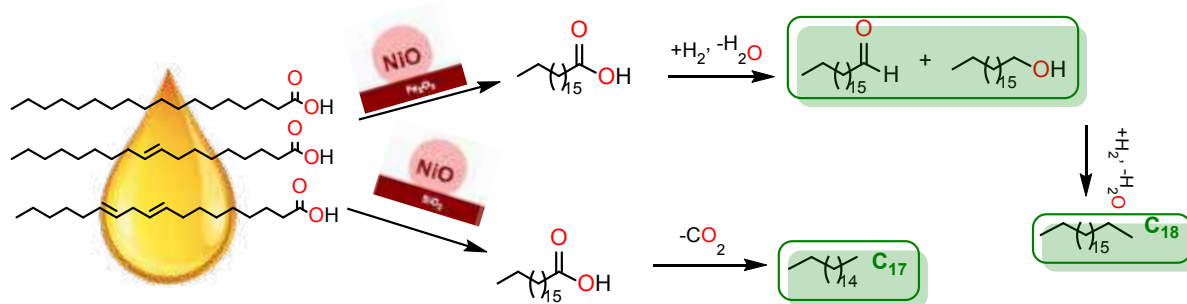
^aResearch Centre for Synthesis and Catalysis, Department of Chemical Science, University of Johannesburg, Auckland Park 2006, South Africa

*Corresponding author: bmakhubela@uj.ac.za

Abstract

The conversion of renewable biomass, particularly triglyceride-derived fatty acids, into sustainable diesel-range hydrocarbons presents significant potential for green fuel technology. Traditional methods, such as hydrodeoxygenation and decarboxylation, commonly require harsh reaction conditions, including high hydrogen pressures. Consequently, developing effective catalytic systems for fatty acid deoxygenation under milder conditions is crucial.

This study explored a novel catalytic approach involving formic acid-mediated hydrogenolysis of stearic acid using nickel and iron catalysts. Specifically, Fe_2O_3 , $\text{NiO}/\text{Fe}_2\text{O}_3$, and $\text{NiO}/\text{SBA-15}$ catalysts were evaluated for their efficacy in selectively producing diesel-range hydrocarbons and oxygenated intermediates.



The catalytic evaluation demonstrated distinct selectivity profiles influenced by the metal-support interaction. Notably, the $\text{NiO}/\text{SBA-15}$ catalyst facilitated efficient decarboxylation, yielding diesel-range hydrocarbons (91% yield, $\text{C}_{14}\text{-C}_{18}$) with up to 157 h^{-1} turnover frequency (TOF). In contrast, Fe-based catalysts (Fe_2O_3 and $\text{NiO}/\text{Fe}_2\text{O}_3$) exhibited superior hydrogenolysis capability, selectively producing oxygenated hydrocarbons, predominantly fatty alcohols and aldehydes (~65% yield), with $\text{NiO}/\text{Fe}_2\text{O}_3$ showing a significantly higher TOF of 630 h^{-1} .

These findings underscore the importance of catalyst composition and metal-support interactions in steering reaction pathways for biomass valorization and further contribute valuable insights into sustainable and economically viable catalytic processes essential for advancing green-diesel technologies.

Keywords: fatty acid, decarboxylation, green diesel, fatty alcohols, fatty aldehydes, nonadecanone, bio-hydrocarbons.

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TECHNO-ECONOMIC ANALYSIS OF PLASTIC WASTES FAST PYROLYSIS TO HYDROCARBONS

**Georgios Iakovou^{a,*}, Antigoni Margellou^a, Petros Soldatos^a, Stylianos Torofias^a,
Konstantinos Triantafyllidis^{a,b,c}**

^aDepartment of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece.

^bChemistry Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

^cInterdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

*Corresponding author: iakovou_y@yahoo.gr

Abstract

Plastic waste crisis has increased interest in alternative waste management strategies that provide environment and economic benefits. The approach of plastic-to-fuel (PTF) aims to valorize plastic waste to valuable liquid and gaseous fuel through thermochemical processes such as pyrolysis, gasification and hydrogenolysis^{1,2}. Techno-economic viability is important for adopting PTF in a realistic industrial scale. In this study, experimental data are presented as well as process design in Aspen Plus of an industrial size plant for the production/isolation of hydrocarbons derived via the pyrolysis of plastic wastes.

Regarding the experimental part, fast pyrolysis was performed in a fixed-bed reactor under inert atmosphere, at 450°C using low-density polyethylene (LDPE). The pyrolysis resulted in three fractions: gases (3.5 wt.%), liquid oil (5.5 wt.%) and high molecular weight hydrocarbons (solids/waxes, 85.6 wt.%). The analysis of gases showed the formation of C₁-C₅ paraffins and olefins, while the liquid oil and waxes are enriched in diolefins, olefins and n-paraffins with carbon number higher than approximately C₁₆. Furthermore, the addition of low-cost catalysts with tuned acidic properties induced cracking of waxes and an increase of liquid oil up to 60 wt.%, composed mainly by olefins within the gasoline fuel range. By estimating the capital expenditure (CAPEX) and operational expenditures (OPEX) of the plant using bibliographical data³, economic indices of the investment, such as ROI and NPV, have been calculated to examine the viability of a potential investment. Results showed the potential of PTF valorization by means of fast pyrolysis. While PTF provides a promising solution to manage plastic waste and reduce fossil fuel dependence, challenges such as relatively high capital costs, feed and product quality stability and regulatory uncertainty are hindering, at the moment, factors.

Keywords: plastic wastes, pyrolysis, hydrocarbons, techno-economic analysis.

Acknowledgements

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CATALYSIS AT THE HEART OF A TERPENE BASED BIOREFINERY

Professor Steven Bull

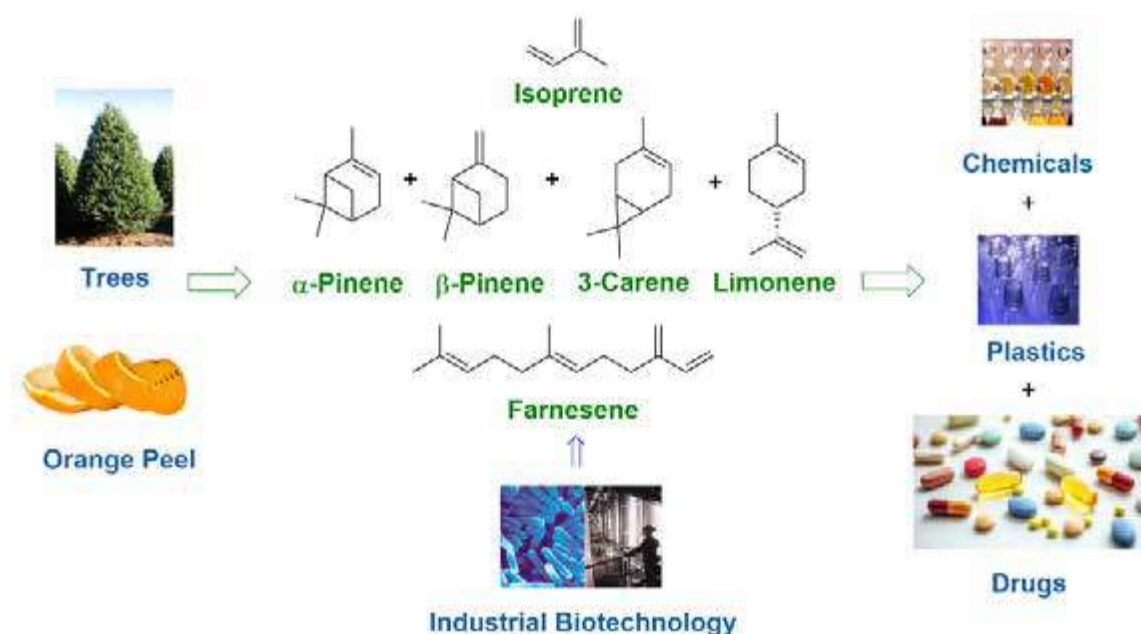
School of Chemistry, University of Leicester, University Road, Leicester, LE17RH

**Corresponding author: sdb45@leicester.ac.uk*

Abstract

Monoterpenes are a class of biorenewable feedstock whose unsaturated hydrocarbon skeletons are well suited for the industrial syntheses of many chemicals that are currently made from non-renewable petrochemical feedstocks. This presentation will describe how catalytic processes can be used to establish a terpene based biorefinery for the synthesis of biorenewable versions of commercially important platform chemicals, polymers, insect repellents and drugs. It will include discussions of acid catalyzed ring-opening reactions,¹ efficient batch and flow catalytic epoxidation protocols,^{2,3} and use of catalytic aromatization reactions to produce benzenoid ring systems.⁴ Sustainable scalable routes to convert different terpene feedstocks into biorenewable versions of polyethylene terephthalate (PET),⁵ paracetamol (acetaminophen),⁶ ibuprofen (Advil)⁶ and all eight stereoisomers of p-menthane-3,8-diol (PMD) will be described. The potential of using terpene derived 4-hydroxyacetophenone as a drop-in feedstock replacement to produce sustainable aromatic products will also be discussed within a terpene biorefinery context.⁷

Keywords: terpenes; biorenewables; catalysis; biorefinery; organic synthesis.



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METAL FREE VISIBLE LIGHT INDUCED CONSTRUCTION OF MULTI NITROGEN HETEROCYCLE COMPOUNDS FROM AZOBENZENE WITH DIBORON ESTER

Xinluo Song, Yu Wang, Yanqi Chen, Subin Hao, Mingde Li a,* , Li Danga,*

^aDepartment of Chemistry and Key Laboratory for Preparation and Application of Ordered Structural Materials of Guangdong Province, Shantou University, Guangdong 515063, China

**Corresponding author: mdli@stu.edu.cn; ldang@stu.edu.cn*

Abstract

Although azobenzene compounds have been widely used in the construction of nitrogen azocyclic compounds¹, the electronic structure and chemical synthesis based on cis azobenzene have not been paid much attention to. Because cis azobenzene is not as stable as trans azobenzene and tends to isomerize rapidly to trans azobenzene under visible light, cis azobenzene based research is often neglected. Our study of the electronic structure of cis and trans azobenzene shows that the highest occupying molecular orbital in cis azobenzene is mainly composed of p orbitals occupied by lone pair electrons of nitrogen atoms, and the interaction between the electron-deficient metal d orbital or the empty p orbital of diboron ester can stabilize the cis azobenzene molecule and further transform it into nitrogen heterocyclic compounds with great practical significance, which will induce a new method of constructing nitrogen heterocycles using azobenzene². Utilizing the interaction between diboron ester and cis azobenzene molecule³, we have preliminarily obtained cis azobenzene vis photoisomerization under visible light. Due to higher reactivity of cis azo bonds, the cyclization reaction of ortho substituted azobenzene (Figure 1) has been achieved, and important compounds such as indole, indazole, and triazole for drug synthesis or organic material preparation have been obtained.

Keywords: Photosynthesis; Heterocycle compounds; Green chemistry; Metal free; Visible light

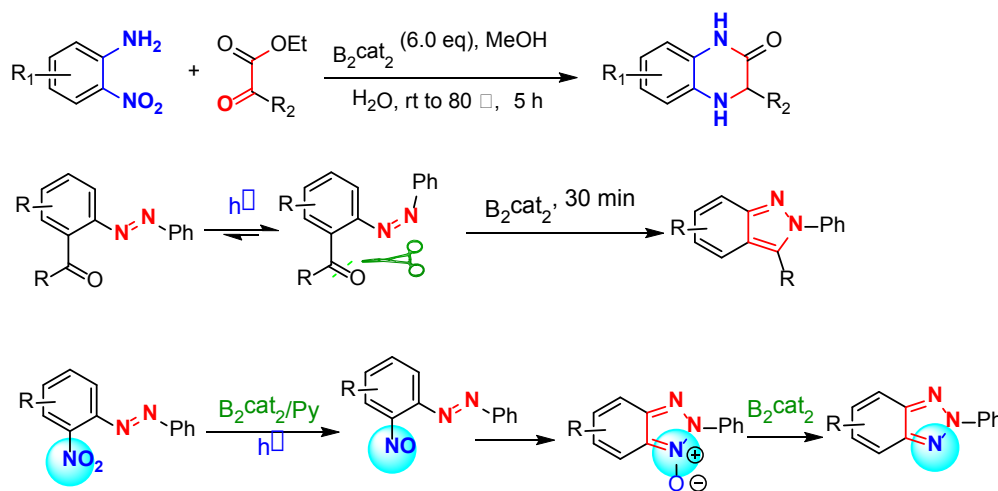


Figure 1. Boron ester mediated synthesis of nitrogen heterocycle compounds.

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PREDICTION OF NUTRIENTS AND PROXIMATE COMPOSITIONS IN AGRICULTURAL CROPS USING NEAR INFRARED REFLECTANCE SPECTROSCOPY

Irna Syairina Sahari^{a*}, Margaret Abat^a, Syazwani Bakar^a

^aAgriculture Research Centre Semongok, Department of Agriculture Sarawak,
KM 20, Borneo Heights Road, 93250 Kuching, Sarawak, Malaysia.

*Corresponding author: irna.rina@sarawak.gov.my

Abstract

Near infrared reflectance spectroscopy (NIRS) is a rapid, non-destructive, cost-effective and deemed environmental-friendly method compared with the conventional chemical analyses method. The NIRS technique was successfully used in the estimation of protein in cowpea leaves¹, chlorophyll and nitrogen in apple² and quality evaluation of sweet potato³. Nevertheless, information on the use of NIRS technique to predict nutrient contents and proximate compositions simultaneously in agricultural crops in tropical region is still limited. We attempted to develop a robust and reliable method to predict quality attributes of food crops in Sarawak using NIRS. A total of 359 food crops and plant materials were scanned with the wavelength ranging from 400 nm to 2500 nm and analysed using WinISI software. A modified partial least-squares regression with cross-validation was used to evaluate the models and identify possible spectral outliers. The calibration equations indicated that NIRS technique has a good to excellent predictive capacity for nitrogen, phosphorus, potassium, calcium, magnesium, iron, zinc, boron, ash, crude fibre, crude protein, ash, total fat, ascorbic acid, acidity and carbohydrate in the tested samples, with the R_c^2 values ranging from 0.8586 to 0.9937. The calibration models for elements such as manganese and copper gave unsatisfactory values. For manganese, the R_c^2 value was 0.5477, and for copper, the R_c^2 was 0.3096, indicating a possible wide variation in the concentrations of those elements in the selected samples. More samples are required to improve the calibration models and increase the accuracy of the prediction capacity. Our findings suggest that NIRS technique may become a preferred method in the future compare with the chemical analyses for predicting nutrients and proximate compositions in agricultural crops and other samples.

Keywords: Non-destructive, simultaneous, environmental, agriculture

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HIGH-ENTROPY NANOMATERIALS FOR ELECTROCATALYTIC WATER SPLITTING

Zhenlong Wang^a, Haibin Zhu^{a*},

^a School of Chemistry and Chemical Engineering, Southeast University

*Corresponding author: zhuhaibin@seu.edu.cn

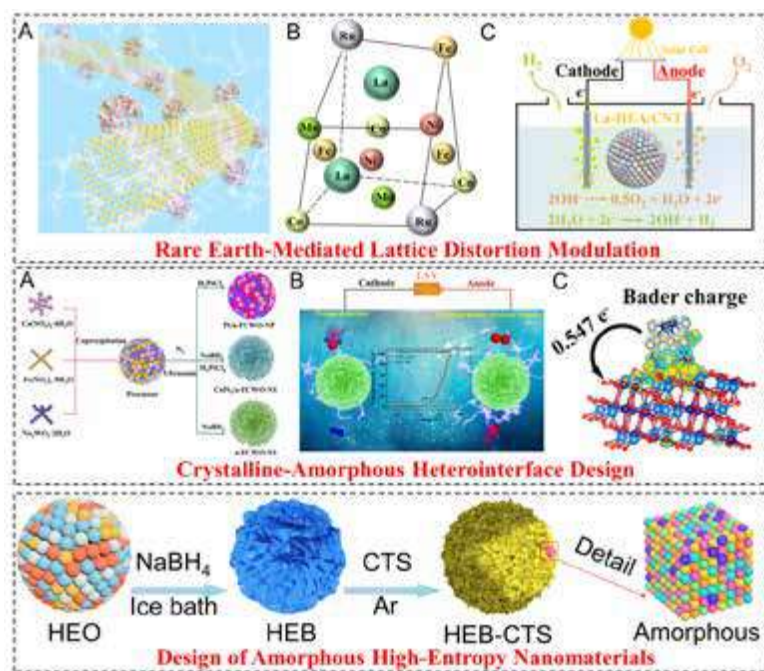
Abstract

High-entropy nanomaterials demonstrate remarkable advantages in electrocatalysis due to their unique multi-element synergy, tunable electronic structures, and exceptional stability. Their multi-site synergistic mechanisms are particularly suitable for multi-step catalytic systems, offering innovative solutions to overcome the limitations of conventional catalysts in complex reactions. Our study develops non-noble and low-noble metal high-entropy electrocatalysts for efficient water splitting, focusing on optimizing intermediate adsorption energies and enhancing active site stability. Three design strategies are implemented:

1. Rare-earth doping induces lattice distortion to modulate d-orbital electrons.¹
2. Amorphous-crystalline heterointerfaces enhance charge transfer.²
3. Design of amorphous high-entropy nanomaterials.³

The optimized catalyst FeCoNiMnRuLa/CNT exhibits superior performance to commercial RuO₂ and Pt/C in alkaline media (1.52 V < 1.53 V@10mA/cm²). Mechanistic studies reveal that lattice distortion and interfacial charge redistribution critically regulate reaction kinetics. Future work will employ in-situ surface reconstruction and coordination microenvironment engineering to further enhance system durability.

Keywords: high-entropy nanomaterials, electrocatalytic, water splitting, amorphous structure



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CARBON-ENCAPSULATED Fe NANOPARTICLES IN Fe-N-C ELECTROCATALYSTS FOR EFFICIENT OXYGEN REDUCTION REACTION

Gao-Yuan Huang^a, Hai-Bin Zhu^{a*}

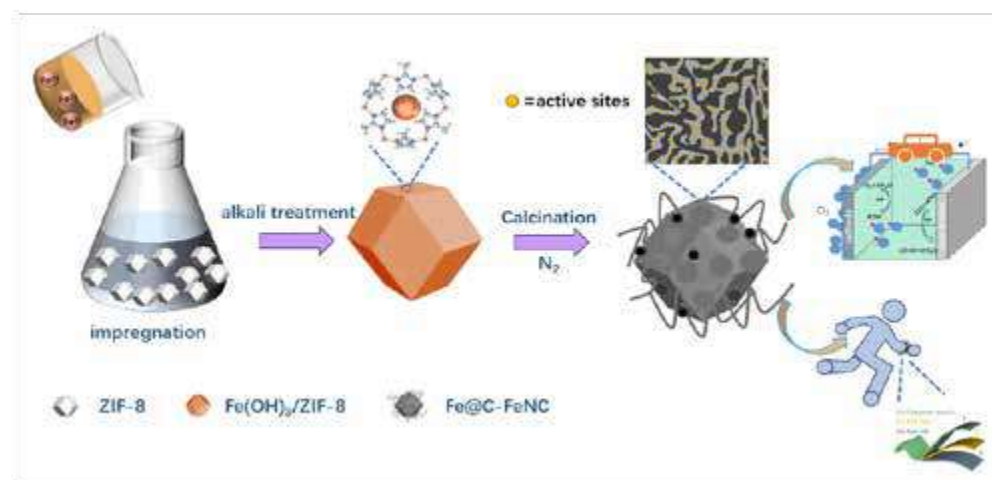
^a School of Chemistry and Chemical Engineering, Southeast University

*Corresponding author: zhuhaibin@seu.edu.cn

Abstract

The global shift toward clean energy alternatives to replace conventional fossil fuels has emerged as an inevitable imperative. Among promising candidates, zinc-air batteries and fuel cells have garnered substantial research interest as next-generation electrochemical energy storage systems. Particularly, the oxygen reduction reaction (ORR) at the cathode serves as the pivotal process in energy conversion devices. The current strategic direction of our laboratory centers on the rational design of Fe-N-C-based electrocatalysts that combine economic viability with superior performance characteristics, aiming to replace traditional noble metal catalysts¹⁻³. However, developing facile and scalable synthetic routes to construct catalysts with well-defined hierarchical porosity continues to pose substantial challenges. Here, we develop a straightforward self-sacrificial templating strategy that addresses three key limitations of existing methods: (i) procedural complexity, (ii) elevated production costs, and (iii) environmental impact. The resulting material, featuring carbon-confined Fe nanoclusters and anchored Fe single-atom sites on porous carbon scaffolds, demonstrates remarkable advantages in enhancing both the activity and stability of the oxygen reduction reaction (ORR) in alkaline media. The optimized catalyst Fe@C-FeNC delivers a high power density of 135 mW·cm⁻² in the self-made zinc-air battery, surpassing the benchmark Pt/C catalyst (90 mW·cm⁻²). This work opens up new opportunities for optimizing the intrinsic activity of Fe-N_x active sites, and designing advanced platinum-group-metal (PGM)-free catalysts for critical energy conversion and storage devices.

Keywords: self-sacrificial templating, hierarchical porous structure, oxygen reduction reaction, zinc-air batteries



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IMPACTIVE: EUROPEAN MECHANOCHEMISTS DEVELOP GREENER PHARMACEUTICALS

Evelina Colacino^{a,*}, Juan José Sáenz de la Torre^b,
Leyre Flamarique^b, Fernando Gomollon-Bel^b.

^aICGM, Univ Montpellier, CNRS, ENSCM, 34293 Montpellier, France.

^bAgata Communications, Santander, Spain.

*Corresponding author: evelina.colacino@umontpellier.fr

Abstract

Mechanochemistry uses mechanical force to drive chemical reactions. In the past few years, this field has experienced a resurgence in Europe, in part thanks to the support of EU-funding bodies to different collaborative initiatives and networks,¹ but also thanks to the additional awareness about the environmental impact of chemistry.² In 2022, the international project IMPACTIVE kicked off with a clear goal: making mechanochemistry a manufacturing reality in pharma. The most optimistic predictions expect an 85% reduction in the ecotoxicity of pharmaceutical production, including a significant reduction of energy consumption and carbon emissions, as well as production costs. With almost €8 million in funding from Horizon Europe, IMPACTIVE gathers 17 partners, including key industries like Merck and Novartis, to ensure efficient technology transfer and early-adoption of the green chemistry and mechanochemistry solutions developed. The poster will present the overall goals of the project, which include the implementation of scalable mechanochemical methods (ball milling, extrusion, resonant acoustic mixing) to make the synthesis of antidiabetic, antihypertensive and anticancer drugs as well as formulation greener, in line with the 12 principles of green chemistry^{3,4} and the United Nations Sustainable Development Goals.⁵ Additionally, the move to mechanochemistry will contribute to solving the supply chain shortage problems, improving the production of drugs during emergencies. The IMPACTIVE project will contribute to the chemistry community in Europe with innovative green synthetic methodologies and catalyse commercialisation.

This project has received funding from the European Union's Horizon Europe Research and Innovation programme (European Health and Digital Executive Agency, HeDEA) under grant agreement No 101057286 (Innovative Mechanochemical Processes to synthesize green **ACTIVE** pharmaceutical ingredients, IMPACTIVE)

Keywords: Mechanochemistry, Green Chemistry, Pharmaceuticals, Sustainability.

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DOPING OF ZN INTO CeO_2 NANOROD AN EFFICIENT CATALYST FOR THE CO_2 CARBONYLATION WITH AMINE REACTION

Nagendra Kulal^a, Yahaya Muhammad Abdullahi^b, Bassam El Ali^{ab}

^aInterdisciplinary Research Center for Refining and Advanced Chemicals,

King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

^bChemistry Department, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

e-mail presenting author: nagendra.kulal@kfupm.edu.sa

Abstract

Carbon dioxide (CO_2) is a significant greenhouse gas that has been identified as a major contributor to global warming and climate change. Carbon dioxide is a non-toxic and readily accessible gas that may be used to make a variety of products, including cyclic carbonates, carbamates, urethanes, substituted ureas, organic carbonates, methanol, and hydrocarbons. One such key transition is the cycloaddition of CO_2 and ethanolamine to produce cyclic carbamate. The primary objective of this work is to develop a catalyst that is both stable and active and has high selectivity for the direct synthesis of 2-oxazolidinone from CO_2 and ethanolamine. The Zn_xCeO_2 nanorod exhibits a higher number of oxygen vacancies in comparison to the cubic and nanorod shapes of CeO_2 . These oxygen vacancies may stabilize the CO_2 molecule by filling one of its oxygen atoms, hence improving catalytic efficacy. Zn/CeO_2 nanorods catalyst show significantly more activity for 2-oxazolidinone synthesis from CO_2 and ethanolamine, as Zn improves CeO_2 surface reducibility. We extensively characterized catalysts to understand their physicochemical properties and correlation with catalytic activity. Under optimum reaction condition 93.7% of ethanolamine conversion and 97.8% selectivity for 2-oxazolidinone were achieved.

Keywords: CO_2 carbonylation, oxide catalyst, carbamate, substituted urea, cyclicurea

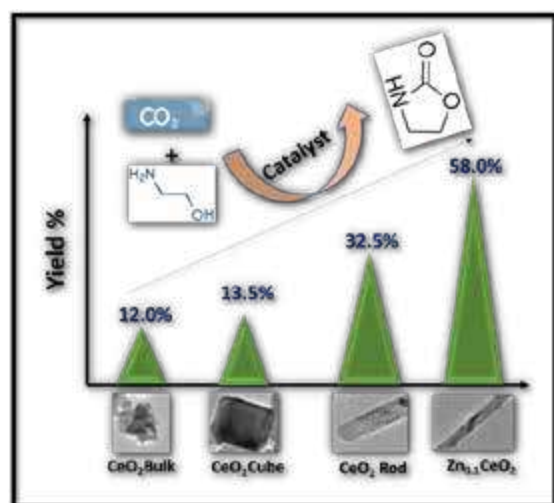


Figure1. Effect of catalyst morphologies and metal doping for catalytic activity

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HYDROGEN-FREE DEOXYGENATION OF MICROALGAE OIL TO PRODUCE SUSTAINABLE AVIATION FUEL

Wei Chun Tung^{a,*}, Wai Kit Tang^b, Joon Ching Juan^{a,*},

*a Nanotechnology & Catalysis Research Center (NANOCAT), IPS Building, Institute for Advanced Studies (IAS),
Universiti Malaya, 50603 Kuala Lumpur, Malaysia.*

b Department of Chemistry, Faculty of Science, Universiti Malaya, Kuala Lumpur, 50603, Malaysia.

**Corresponding email: jcjuan@um.edu.my*

Abstract

As the global aviation industry seeks to reduce its carbon footprint, the development of sustainable aviation fuel (SAF) has become a critical priority. Sustainable aviation fuel (SAF) is recognised as a key solution to decarbonize aviation, a sector responsible for approximately 2-3% of global CO₂ emissions (IATA, 2022). However, the common commercial SAF process which hydroprocessed esters and fatty acids consumes hydrogen gas, and the commercial production of 1 kg hydrogen will produce approximately 9.7 kg of CO₂, which defeats the integrity of SAF (Dutta, 2024). Alternative such as green hydrogen will significantly increase the cost of SAF (Kumar, 2023). This study explores catalytic deoxygenation *without* hydrogen input to convert microalgae oil into SAF-compatible hydrocarbons. Using Ni/SiO₂ at 320°C under inert Ar, with ethyl laurate as a model compound, oxygen was removed as CO₂/CO without external H₂, achieving 80% conversion and 50% hydrocarbon yield (C₁₁ alkanes). We conclude that hydrogen-free deoxygenation enables cost-efficient, scalable SAF production, reducing reliance on H₂ infrastructure while significantly lowering carbon footprints to support aviation decarbonization.

Keywords: sustainable aviation fuel, hydrogen-free deoxygenation, renewable hydrocarbons, renewable energy, biomass conversion.

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MITIGATING ABSOLUTE HUMIDITY CHALLENGES IN AMBIENT- PROCESSED CSPBI₃ PEROVSKITE SOLAR CELLS: TRIPHENYLPHOSPHINE- BASED ADDITIVES FOR TROPICAL CLIMATES

Whui Dong Wong^a, Bao Lee Phoon^a, Joon Ching Juan^{a*}, Lai Chin Wei^a,
Nurhidayatullaili Muhd Julkapli^a

^a Nanotechnology & Catalysis Research Center (NANOCAT), Institute for Advanced Studies, Advanced Studies
Complex, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.

*Corresponding email: jcjuan@um.edu.my

Abstract

Inorganic CsPbI₃ perovskite solar cells (PSCs) offer enhanced thermal stability but face severe phase instability under ambient processing, particularly in tropical climates where high absolute humidity (AH >20 g/m³, 30°C) accelerates the degradation of photoactive black-phase CsPbI₃ to a non-perovskite yellow phase. Unlike conventional relative humidity (RH) studies, this work investigates the role of absolute humidity, a critical yet overlooked factor in tropical regions like Malaysia on CsPbI₃ phase dynamics. We introduce triphenylphosphine (TPP) and its halogenated derivatives (Cl/F-TPP) as dual-functional additives to simultaneously (1) stabilize the black-phase CsPbI₃ via strong P→Pb coordination at grain boundaries and (2) mitigate moisture ingress through hydrophobic aryl and halogen moieties. By correlating AH levels (15–30 g/m³, 25–30°C) during ambient film fabrication with phase evolution, we hypothesized that halogenated TPP additives suppress yellow-phase formation even at extreme AH conditions (25 g/m³, 30°C), retaining black-phase content after 72 hours. Spectroscopic and structural analyses are employed to investigate the role of TPP and halogenated-TPP additives in passivating undercoordinated Pb²⁺ defects through Lewis's acid-base interactions and forming a moisture-resistant surface layer, with the aim of suppressing H₂O adsorption under high absolute humidity (30 g/m³ AH). This study provides a humidity-resilient additive strategy for inorganic PSCs, bridging the gap between lab-scale development and real-world deployment in high-AH tropical environments.

Keywords: Absolute humidity, Ambient processing, CsPbI₃ perovskite, Triphenylphosphine and its halogenated derivatives, Phase stability

QUANTUM CHEMICAL INVESTIGATIONS INTO THE STRUCTURAL AND SPECTROSCOPIC PROPERTIES OF CHOLINE CHLORIDE-BASED DEEP EUTECTIC SOLVENTS

M. Ashraful Hasan,^{1,*} Ismail M. M. Rahman,^{2,*} M. Rithoan Hossain,¹ Faisal Islam Chowdhury^{1,*}

¹Department of Chemistry, Faculty of Science, University of Chittagong, Chattogram 4331, Bangladesh

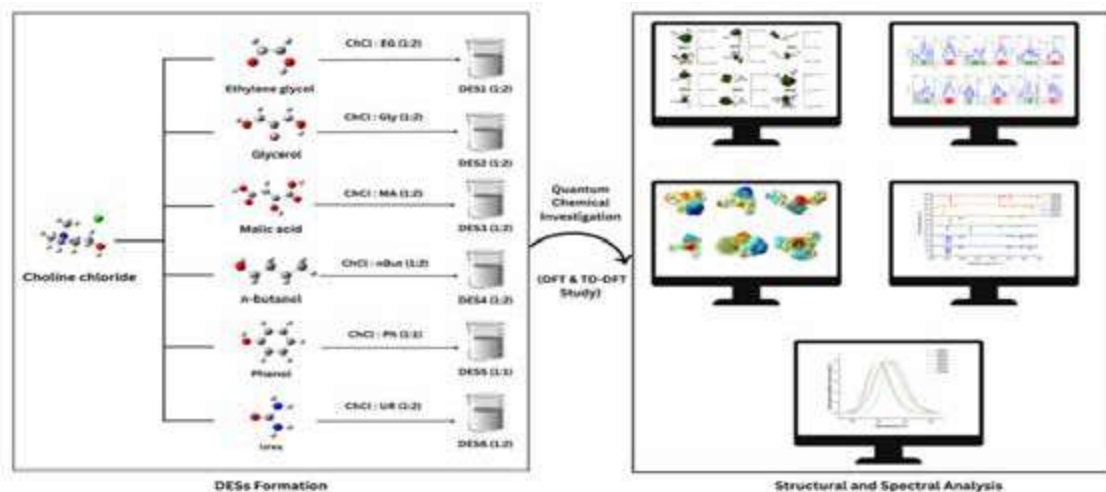
²Institute of Environmental Radioactivity, Fukushima University, 1 Kanayagawa, Fukushima City, Fukushima 960-1296, Japan

*Corresponding author(s): ashrafulhasan.chem.cu@gmail.com (MAH);
immrahman@ipc.fukushima-u.ac.jp (IMMR); faisal@cu.ac.bd (FIC)

Abstract

The chemical process industries are progressively embracing green technologies and sustainable waste management techniques due to growing environmental concerns and the impact of climate change. Deep Eutectic Solvents (DESs), formed by combining neutral molecules (e.g., choline chloride, ChCl) with hydrogen bond donors, have emerged as promising eco-friendly solvents with diverse applications in chemical, pharmaceutical, and separation processes. In this context, modern quantum-based research is focused on eutectic mixtures, particularly those formed by ChCl as a hydrogen bond acceptor with various hydrogen bond donors at specific mole ratios. The properties and validity of these DESs are investigated through density functional theory (DFT) analysis of their molecular dynamics simulations. This quantum computational approach offers valuable insights for designing the desired conductive liquids. Furthermore, the density of states analysis allows for studying the electronic structure and quantifying the number of states occupied per unit of energy. The quantum and vibrational properties of experimentally synthesized DESs are simulated using DFT B3LYP/6-31G(d,p). Current research aims to design and understand the properties of eutectic solvents to develop novel, environmentally benign alternatives for the chemical industry.

Keywords: Eutectic solvents; Quantum calculation; Density Functional Theory; Ionic liquid; Green solvent, Molecular dynamics



BUILDING A GLOBAL, INCLUSIVE COMMUNITY TO TACKLE SUSTAINABILITY

Francesca M. Kerton^{a*}

^a*Department of Chemistry, Memorial University of Newfoundland, Canada.*

^{*}*Corresponding author: fkerton@mun.ca*

Abstract

The Global Conversation on Sustainability was launched in 2022 by IUPAC (International Union of Pure and Applied Chemistry) and IYCN (International Younger Chemists Network) to celebrate and highlight the role that chemistry can play in achieving the UN Sustainable Development Goals.^{1,2} This is an umbrella event that coordinates individual lectures, panel discussions, world cafés, and other formats organized by engaged individuals and organizations worldwide. This event has led to new collaborations between IUPAC, IYCN, and Beyond Benign, and empowered younger chemists around the world. For example, in 2024, IUPAC and Beyond Benign worked together to hold a webinar on sustainable lab practices with Dr. Thomas Freese (University of Gröningen) highlighting activities that can make labs safer and greener through systemic change.³ Similarly, Beyond Benign and the Lab Safety Institute (USA) worked together to enable a conversation on possible safer substitutions of methylene chloride (dichloromethane) by hosting a free webinar and panel discussion. IUPAC's Chemical Research Applied to World Needs (CHEMRAWN) committee has similarly been working on materials to help scientists worldwide engage in systemic change. CHEMRAWN developed an e-waste resource webpage and supported a special issue of Chemistry Teacher International focused on education about e-waste.⁴ A new IUPAC project on Promoting Chemistry Applied to World Needs is currently underway and includes a webinar series in collaboration with Beyond Benign. In addition to webinars and online 'real-time' panel discussions, local safety and sustainability moments in group meetings, or discussion board chats (e.g. Green Chemistry Teaching and Learning Community, GCTLC) can help us all grow as a community, and improve safety and sustainability in an inclusive way.

Keywords: Sustainability, Green Chemistry, Education, Safety, Outreach



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ENGAGING LEARNERS THROUGH THE BENEFITS AND CHALLENGES OF PLASTICS TOWARDS ACHIEVING THE UN SDGs

Jane E. Wissinger^{a,*}

^aUniversity of Minnesota, Minneapolis, MN, United States

*Corresponding author: jwiss@umn.edu

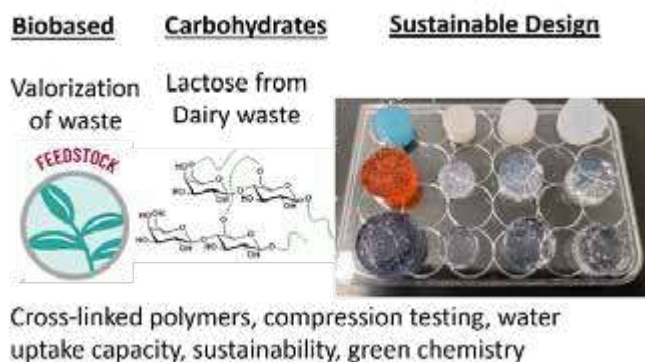
Abstract

In a little over a hundred years, chemists and chemical engineers have developed the field of synthetic organic plastics so that materials of practically any desired function can be made. Humankind has benefited through life-saving prevention of infection and disease (SDG 3), clean water technologies (SDG 6), food preservation (SDG 2) and lightweight materials for affordable and clean energy (SDG 7); for example. However, the unintended consequences of plastic and microplastics pollution are causing devastating harm to the environment and life on the planet. A recent publication demonstrated that plastics use and production are exceeding planetary boundaries limits and is not compatible with a sustainable future.¹

This dilemma presents relatable and engaging topics for students to explore in the context of chemistry and a socio-environmental sustainability problem. This presentation will share instructional tools for illustrating green chemistry as a toolbox for design of sustainable plastics using a graphical Sustainable Polymer Framework (SPF).² Inherently, a systems approach to understanding each pillar (feedstock, process, intended use, and end-of-use) and their interconnected systems provides connection to many of the UN SDGs, including but limited to, responsible consumption and production (SDG 12), climate action (SDG 13), and life below water (SDG 14). Incorporation of this curriculum into introductory chemistry lecture and laboratory courses will build awareness across their multi-disciplinary student population and inspire chemistry majors in upper division classrooms with the role chemistry will play in sustainable development.

In concluding the talk, data from the Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD) study will be presented that illustrates how IUPAC projects across divisions and committees are advancing sustainable development toward the 2030 Goals. Together, we can make strides for people, planet, and prosperity.

Keywords: chemistry education, systems thinking, UN SDGs, green chemistry, sustainable plastics



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FROM TRASH TO SUDS: TANDEM UPCYCLING OF WASTE POLYOLEFIN PLASTICS TO DETERGENTS

Zhen Xu^{a,b*}, Rong Yang^a,

^a School of Chemistry and Chemical Engineering, Northwestern Polytechnical University, Xian, China.

^b Shandong Scitech Innovation Group Co., Ltd, Jinan China.

*Corresponding author: zhenl@nwpu.edu

Abstract

Polyolefin waste represents an underutilized resource for synthesizing high-value chemicals, providing a sustainable alternative to petroleum-based production. Our recent studies have successfully transformed polystyrene (PS) into pharmaceutical intermediates and fragrance compounds through tandem catalytic processes, achieving magnitude value improvement.^[1,2] For polyethylene (PE) and polypropylene (PP), the dominant polyolefin types, surfactant production emerges as an economically compelling target. Market analysis reveals surfactants hold at least twofold higher value than virgin plastics, fuels, or BTXs (benzene, toluene, xylenes), coupled with comparable market capacity and expanding global demand. However, technical barriers persist in converting post-consumer PE and PP wastes into surfactants, particularly regarding reaction kinetics control, product uniformity, and process robustness when handling contaminated real-life wastes from supply chains. This discussion highlights our recent advancements in overcoming these obstacles. By integrating tandem strategy with reactor engineering, we have achieved controlled conversion of polyolefin waste into surfactants.^[3,4] Case study shows that surfactants derived from real-life polyolefin waste in China can rival commercial surfactants in terms of foaming performance, biodegradability, and detergency, while outperforming petroleum-based processes in both economic and ecological impact.^[4] By focusing on scalability and economic feasibility, our work paves the way for practical plastic upcycling, contributing towards a more sustainable future.

Keywords: Polyolefins, real-life plastic wastes, upcycling, detergents



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CASE STUDY FOR PROMOTING POSITIVE RESEARCH AND EDUCATION

**Tien Thuy Quach^{a,b*}, Affiong Iyire^a, Daniel Burrell^a, Radeyah Ali^a, Dan Rathbone^a,
Afzal Mohammed^a, Daniel Kirby^a**

^a *Aston Pharmacy School, College of Health & Life Sciences, Aston University, Birmingham, B4 7ET, United Kingdom.*

^b *International Younger Chemists' Network (IYCN), International Union of Pure and Applied Chemistry (IUPAC).*

**Corresponding author: T.Quach@aston.ac.uk*

Abstract

Although the international postgraduates (i.e. 1-year Post-Taught-Graduates) take up a larger portion and faster return on investment in the UK's higher education and employment, there is still limited support and funding for them during and after Covid-19 pandemic. As a case study, Aston University has different actions aligning well with the Sustainable Development Goals (SDGs) to facilitate those students. Firstly, Aston Pharmacy School successfully launched novel teaching laboratories and established the interactive industrial site visits for all postgraduates ^[1]. In recent years, all MSc students could access the forefront of combining cutting-edge technologies and data analytics thanks to the industrial companies in chemical, analytical, pharmaceutical sciences and related fields. Besides, our team could organize several practical events such as "Journal Club", "Global Conversation on Sustainability" to discuss and apply good practice across multiple institutions beyond the UK ^[2]. After that, the academic and technical staff across 3 courses (i.e. MSc Drug Delivery, MSc Pharmaceutical Sciences, and MSc Pharmacokinetics) can be able to specify and apply appropriate sustainable materials and processing when supervising MSc student projects. One of our recent achievements was offering innovative development grants every year to support at least 12 pharmacy students and technicians to present their research and works in the international/national conferences, trainings, etc ^[3,4]. We frequently introduce several activities-fundings from International Younger Chemists' Networks (IYCN) to all postgraduates for their personal and professional development. We also kicked off new workshop series "Widening Positive Impacts" (funded by RSC and SYSCOedu) to feature many inspiring life-changed stories ^[5]. In conclusion, our works marked a new chapter for international postgraduates to become more accessible to industrial experiences, more motivated to sustainable research, and more determined to showcase relevant outputs. This systematic change can accelerate more skillful postgraduates to be ready for work and life at their early stages.

Keywords: industrial site visits, novel teaching laboratories, innovative development grants, IYCN's activities-fundings, new workshop series.

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**53rd International Union of Pure & Applied Chemistry General Assembly (IUPAC 2025)
and 50th World Chemistry Congress (50WCC)**

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QUANTUM DOTS-BASED BIOSENSOR FOR FOOD PATHOGEN DETECTION

Jaafar Abdullah^{1,2}

¹*Institute of Nanoscience and Nanotechnology, University Putra Malaysia, 43400 Serdang, Selangor, Malaysia*

²*Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia*

Corresponding author: jafar@upm.edu.my

Abstract

The detection of foodborne pathogens is critical for ensuring food safety and agricultural productivity. Quantum dots (QDs), particularly carbon quantum dots (CQDs), have emerged as promising nanomaterials for biosensing applications due to their exceptional optical properties, biocompatibility, and stability. CQDs offer tuneable fluorescence, high quantum yield, and excellent water solubility, making them suitable for pathogen detection through DNA interaction and immunoreaction mechanisms. This study focuses on the development of a CQDs-based biosensor for the detection and monitoring of *Escherichia coli* O157:H7 (*E. coli* O157:H7), a major foodborne pathogen that threatens human health, and *Xanthomonas oryzae* pv. *Oryzae* (Xoo), rice bacterial leaf blight disease in rice leaf for agricultural applications. The biosensor operates by functionalizing CQDs with specific DNA probes, enabling high-affinity binding with *E. coli* O157:H7 via hybridization with target genetic sequences, which induces fluorescence signal changes that allow for sensitive and selective pathogen detection. While antibodies against Xoo bacterial cells are conjugated with CQDs and gold nanoparticles serving as bio-probes to initiate an immunoreaction between antibodies and target cells led to immuno-aggregation complex, triggering fluorescence signal changes. Furthermore, this study offers a new opportunity for nanomaterial-based optical DNA and immunoassay with advanced use of carbon quantum dots for prospective diagnostic of food safety and early screening of rice bacterial leaf blight disease in agricultural applications. The integration of CQDs-based biosensors with portable detection platforms can provide real-time monitoring capabilities, enhancing food safety and agricultural protection. This work underscores the potential of CQDs as an innovative and efficient biosensing platform for pathogen detection, offering a rapid, cost-effective, and highly sensitive alternative to conventional microbiological techniques. Future research should prioritize enhancing sensor performance, expanding field applicability, and developing multi-target detection capabilities to advance biosensors for comprehensive health diagnostics and agricultural monitoring.

Keywords: Carbon quantum dots, biosensor, DNA interaction, immunoreaction, pathogen

FEEDING THE FUTURE: STRATEGIC PATHWAYS TO ACHIEVING ZERO HUNGER

Wickneswari R.

Nomatech Sdn Bhd., TGB-01, Block B, UKM-MTDC Technology Centre, 43650 Bangi, Selangor.

**Corresponding author: wicki@nomatech.com.my*

Abstract

Achieving zero hunger (SDG2) requires resilient food systems that ensure equitable access to nutrition while safeguarding environmental sustainability. Innovative global and regional strategies, include hydroponics, blockchain-powered food distribution, and food waste reduction. Strengthening local food security depends on academia-industry partnerships that drive agricultural innovation, improve supply chain efficiency, and scale sustainable farming solutions. Universities play a critical role in advancing research on climate-smart agriculture, precision farming, and biotechnology, while industry collaborates to commercialize these technologies, enhance market accessibility, and support smallholder farmers. By integrating science-driven policymaking, corporate investment in sustainable food production, and grassroots community efforts, we can develop robust, inclusive food systems. Challenges include resource limitations, adopting barriers and policy gaps whilst there are opportunities for cross-sector collaboration to create a hunger-free future.

Keywords: Food and nutrition security, climate-smart agriculture, food systems, food waste reduction.

FROM FLOCK TO FORK: POULTRY WELFARE AND FOOD SAFETY FOR A SECURE FUTURE

Zulkifli Idrus

Universiti Putra Malaysia

**Corresponding author: zulidrus@upm.edu.my*

Abstract

As global demand for poultry rises, animal welfare and food safety are increasingly recognised as interconnected priorities in building a sustainable food system. Consumers today are not only concerned about how much food is produced but also how it is raised, how safe it is, and its impact on public health. This paper examines how welfare-focused poultry production can play a pivotal role in enhancing food safety and ensuring long-term food security. Animal welfare is increasingly recognised for its impact on both food quality and food safety. Stressful conditions not only reduce meat quality but also impair immune function and disrupt gut microbiota, leading to increased colonisation and shedding of foodborne pathogens. Advancements in management, feeding, and housing practices not only improve animal well-being but also reduce the prevalence of foodborne pathogens and limit the need for antimicrobials, thereby addressing the growing threat of antimicrobial resistance (AMR). In contrast, poor welfare conditions are closely linked to increased disease susceptibility, compromised immunity, and elevated food safety risks. By embracing a holistic “flock to fork” perspective, the poultry industry can contribute meaningfully to a food system that is not only productive but also safe, ethical, and resilient for future generations.

ADVANCING FOOD SECURITY IN MALAYSIA THROUGH SUSTAINABLE AGRICULTURE

**Christopher John Biai, Norimah Binti Jumat, Nadea Binti Muhammed Nordin &
Mohd Sobri bin Ismail**

Crop Industry Development Division, Department of Agriculture

**Corresponding author: christopherjb@doa.gov.my*

Abstract

The issue of hunger is becoming increasingly critical, exacerbated by ongoing global challenges such as pandemics, climate change and armed conflicts. These factors contribute to rising food insecurity worldwide. It is estimated that by 2030, more than 600 million people worldwide will face hunger if urgent action is not taken. Under SDG 2: Zero Hunger, the aims are to end hunger, achieve food security, improved nutrition and promote sustainable agriculture.

Malaysia through the Ministry of Agriculture and Food Security has outlined the National Agro-Food Policy 2.0 (DAN 2.0) for the period of 2021 to 2030 which directly supports Sustainable Development Goal 2 (SDG 2): Zero Hunger. DAN 2.0 aims to ensure the nation's food supply security through a sustainable, competitive and resilient agricultural system in line with the goal of end hunger and improving food security. Programs and activities that support this goal are Integrated Pest Management (IPM), an approach to pest control that considers ecological and biological factors by combining various methods and practices, Pesticide-Free Agriculture refers to farming practices using natural alternatives or organic methods instead of synthetic pesticides. Biopesticide refers to pesticides derived from natural sources such as plants, bacteria, fungi, animals or minerals. Biofertilizers that utilize natural fertilizers containing living microorganisms that promote the plant growth by enhancing nutrients availability in the soil. Certification programs such as myGAP & myOrganic that were already in place since 2002 is to certify farms with good agricultural practices as well as to certify program focuses on promoting organic agricultural practices and ensuring compliance with organic farming. Finally, Self-Sufficiency Ratio (SSR), an indicator to measures the extent to a country's domestic production meets its own domestic consumption of various food items. All these programs have been contributing to the sustainable agriculture in Malaysia.

The set targets can be achieved through comprehensive implementation strategy, active and inclusive participation from all sectors to ensure a meaningful and lasting impact.

Keywords: Sustainable Development Goal 2, Zero hunger, food security, sustainable agriculture.

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THE FATE AND POTENTIAL IMPACTS OF CHIRAL PESTICIDES IN COMPLEX AGRICULTURAL SOIL ENVIRONMENTS

Hui Liu^{a,*}, Miqi Li^a

^aNortheast Agricultural University, China

*Corresponding author: liuh@neau.edu.cn

Abstract

Developing highly efficient and low toxic chiral pesticide enantiomers is one of the means to reduce environmental pollution, which also requires comprehensive environmental assessment data support. Most of the applied pesticides enter soil environment instead of plants, and their environmental behavior characteristics along with impacts on soil environment are influenced by complex agricultural production materials, which have therefore received widespread attention. We have been studying soil microenvironment safety with the co-existence of two fungicides and three agricultural production materials containing fertilizers, antibiotics, microplastics. Specific composite stress design includes: Zoxamide and fertilizers¹ or antibiotics²; Penthiopyrad and fertilizers³ or microplastics⁴. Present work has proven that fertilizers, antibiotics, and microplastics could alter the half-life and enantioselectivity of two chiral fungicides in soil. Joint stress mostly focused on soil physicochemical properties, nutritional status, enzyme activity, microbial community composition and diversity. Through correlation analysis, it was found that soil ecological indicators were significantly correlated with the dissipation behavior of chiral fungicides, and there were also links between each indicator. Targeting these results, future studies are expected to achieve the following goals: (1) Targeted chiral pesticide monomers with more efficient and low toxicity characteristics will be released referring to comprehensive assessment in complex agricultural soil environments; (2) It is expected to find microbial resources that can promote the degradation of these two chiral fungicides.

Keywords: chiral pesticides, complex joint stress, enantioselective dissipation, soil health, correlation mechanism analysis



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MAXIMIZING SINGLE-CELL PROTEIN YIELD FROM VEGETABLE WASTE VIA OPTIMIZED LIQUID-STATE FERMENTATION: A STEP TOWARDS CIRCULAR BIOECONOMY

Kashif Rasool^{a,*}, Zukhruf Asim^{a,b}, Hafiz Muhammad Aamir Shahzad^a, Khaled A Mahmoud^a,
 Fares Almomani^b,

^a Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University, Qatar Foundation, P. O. Box 34110, Doha, Qatar.

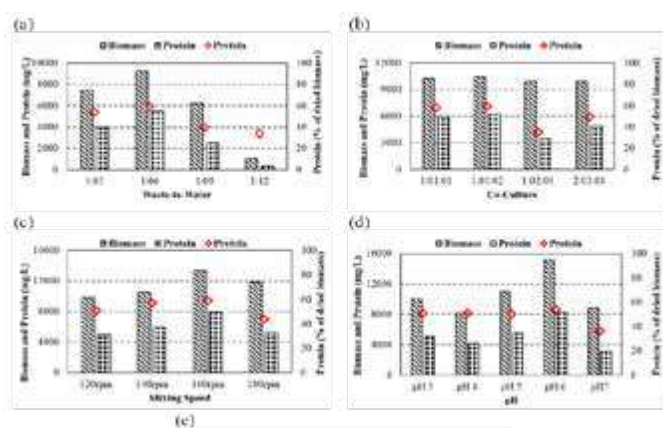
^b Department of Chemical Engineering, Qatar University, Qatar.

*Corresponding author: krasool@hbku.edu.qa

Abstract

Protein-rich animal feed is crucial for supporting the growing global demand for meat, poultry, and aquaculture, yet traditional feed sources such as soybean and fishmeal place a significant burden on land, water, and marine ecosystems. In response to these challenges, the valorisation of agro-industrial waste into alternative protein sources, such as single-cell protein (SCP), offers a promising solution to improve food security and sustainability. SCP, derived from microbial fermentation, presents a viable substitute for conventional feed proteins, reducing reliance on finite resources and minimizing environmental impact. This study examined the use of liquid-state fermentation (LSF) for SCP production from vegetable waste, specifically capsicums, cucumbers, eggplants, and tomatoes. Key operational parameters—such as the waste-to-water ratio, mixing speed, yeast co-culture ratios, pH, and fermentation time—were systematically optimized to maximize SCP yield. Experiments were designed using waste-to-water ratios of 1:3, 1:6, 1:9, and 1:12; mixing speeds of 120, 140, 160, and 180 rpm; yeast co-culture ratios of *Saccharomyces cerevisiae*, *Candida tropicalis*, and *Candida krusei* (1:1:1, 1:1:2, 1:2:1, and 2:1:1); pH levels ranging from 3 to 7; and fermentation times from 2 to 8 days. Optimized parameters were evaluated based on biomass yield, SCP production, and protein content in the dried biomass. The optimal conditions for the highest SCP production were achieved with a waste-to-water ratio of 1:6, a mixing speed of 160 rpm, a pH of 6, and a retention time of 6 days, with a yeast co-culture ratio of 1:2:1. This study emphasizes the significance of optimizing fermentation parameters in LSF and presents a sustainable method for converting vegetable waste into SCP, contributing to both waste valorisation and the production of protein-rich animal feed.

Keywords: Single-cell protein (SCP); Liquid-state fermentation (LSF); Waste valorisation; Protein-rich animal feed; Agro-industrial waste



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DETERMINING OF MOSH AND MOAH IN PALM OIL MATRICES USING ONLINE HPLC-GC-FID ANALYSIS: VERIFICATION OF ISO 20122/2024 METHOD

Maznah Zainol *and Azmil Haizam Ahmad Tarmizi

*Malaysian Palm Oil Board (MPOB), No. 6 Persiaran Institusi, Bandar Baru Bangi, 43000 Kajang, Selangor,
Malaysia*

**Corresponding author: maznahz@mpob.gov.my*

Abstract

Mineral oil saturated hydrocarbons (MOSH) and mineral oil aromatic hydrocarbons (MOAH) are contaminants of concern in palm oil industry due to their lipophilic nature and potential sources of contamination during processing. Currently, the proposed maximum level of MOAH in products containing more than 50% fat or oil is set at 2.0 mg/kg. However, no official limit has been established for MOSH in food products. Therefore, accurate and reliable quantification of these contaminants is essential for regulatory compliance and maintaining product integrity. This study verifies the applicability of the ISO 20122:2024 method for determining MOSH and MOAH in crude palm oil (CPO) using an automated online HPLC-GC-FID system. Optimisation of the on-line LC-GC-FID system, saponification and purification method were conducted to improve the limit of quantification (LOQ) of the method. The method was evaluated for linearity, accuracy, precision, and LOQ to confirm its suitability for routine analysis. Linearity was demonstrated using CyCy and TBB calibration curves for MOSH and MOAH, respectively, with correlation coefficients (R^2) of 0.998 and 0.999. The method achieved a low LOQ of 1.0 mg/kg for both MOSH and MOAH. Recovery rates ranged from 88% to 119% for MOSH and 67% to 122% for MOAH indicating good method accuracy. The performance of the MPOB's laboratory was assessed through inter-laboratory comparisons, with calculated z-scores ranging from -0.16 to 0.33 for MOSH and -0.74 to 0.60 for MOAH. All z-scores were within the acceptable limit ($z\text{-score} \leq 2$), confirming the method's robustness and reliability. These findings establish a standardised and reliable approach for MOSH and MOAH determination in palm oil supporting industry compliance with food safety regulations.

Keywords: Mineral oil saturated hydrocarbons (MOSH); mineral oil aromatic hydrocarbons (MOAH); crude palm oil (CPO); ISO 20122:2024; Online HPLC-GC-FID

DEVELOPMENT AND OPTIMIZATION OF AN ELECTROCHEMICAL BIOSENSOR FOR SENSITIVE DETECTION OF ZEARELENONE IN FOOD SAFETY APPLICATIONS

Nur Azura Mohd Said^{a*}, Norhafniza Awaludin^a, Erna Mutiara Masdek^a

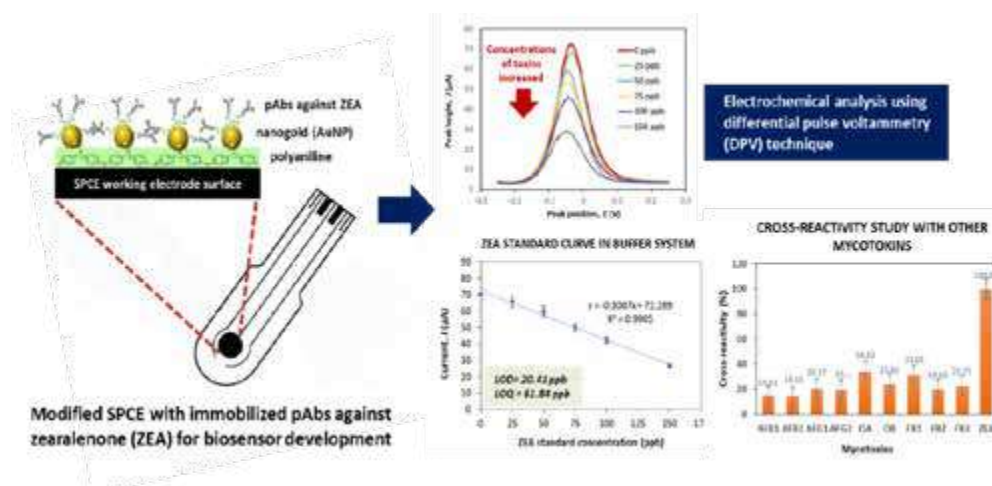
Malaysian Agricultural Research & Development Institute (MARDI)

*Corresponding author: nazurams@mardi.gov.my

Abstract

Zearalenone (ZEA) is a mycotoxin produced by *Fusarium* fungi, commonly contaminating grains and posing health risks to both humans and animals due to its estrogenic effects. Conventional detection methods, such as chromatographic techniques, offer high accuracy but require sophisticated equipment and lengthy processing times. This study presents the development of an electrochemical biosensor for the rapid and sensitive detection of ZEA using a modified screen-printed carbon electrode (SPCE) platform, incorporating anti-ZEA polyclonal antibodies (pAbs) as the biorecognition element. While monoclonal antibodies and aptamers are emerging alternatives, pAbs remain highly relevant due to their ability to recognize multiple epitopes, enhancing sensitivity in complex matrices. Surface modification with polyaniline (PANi) and gold nanoparticles (AuNPs) significantly enhances peak height and reduces peak separation compared to unmodified SPCE. The concentration of immobilized pAbs was optimized, and with 0.05 mg/mL pAbs, a linear standard curve was established in a buffer system, yielding a limit of detection (LOD) of 20.41 ppb and a limit of quantification (LOQ) of 61.84 ppb. A cross-reactivity study confirmed the sensor's specificity, demonstrating minimal interference from other mycotoxins. The developed biosensor offers a promising alternative to conventional methods, providing a portable, cost-effective, and real-time analytical tool for ZEA monitoring in agricultural and food safety applications.

Keywords: electrochemical biosensor, mycotoxins, zearalenone



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BIOFILM FORMATION OF MULTIDRUG-RESISTANT *STAPHYLOCOCCUS AUREUS* ON STAINLESS STEEL SURFACES: INFLUENCE OF TEMPERATURE AND TIME, AND THE EFFICACY OF COMMERCIAL DISINFECTANTS

Nor-Khaizura Mahmud Ab Rashid^{1,2*}, Nur Syifa' Jamaludin¹, Nor Ainy Mahyudin³

¹Department of Food Science, Faculty of Food Science and Technology, Universiti Putra Malaysia, 43400 Serdang Selangor, Malaysia

²Laboratory of Food Safety and Food Integrity, Institute of Tropical Agriculture and Food Security, Universiti Putra Malaysia, 43400 Serdang Selangor, Malaysia

³Department of Food Service and Management, Faculty of Food Science and Technology, Universiti Putra Malaysia, 43400 Serdang Selangor, Malaysia

*Corresponding author: norkhaizura@upm.edu.my

Abstract

Staphylococcus aureus is a pathogenic bacterium capable of forming biofilms on food processing surfaces, leading to cross-contamination in food production. In Malaysia, multidrug-resistant *S. aureus* (MDRSA) has been studied in foodservice environments, but little is known about its survival and biofilm persistence. This study aimed to investigate the biofilm formation of MDRSA on stainless steel surfaces at 25°C and 37°C over 15 days and assess the efficacy of disinfectants in biofilm elimination. A total of 23 MDRSA strains were tested for biofilm formation, while three MDRSA strains were selected for elimination tests using different concentrations of peracetic acid and sodium hypochlorite. Biofilm levels ranged from 3.56 to 6.80 log CFU/mL at 25°C and 3.74 to 7.05 log CFU/mL at 37°C, with SA18 exhibiting the highest biofilm formation on Day 9 at both temperatures. Most MDRSA strains showed stronger biofilm formation at 37°C, their optimal growth temperature. Among the disinfectants, sodium hypochlorite was the most effective, achieving a reduction of 2.48 to 3.54 log CFU/mL across all tested concentrations. In conclusion, MDRSA forms strong biofilms on stainless steel, particularly at 37°C, and sodium hypochlorite is an effective disinfectant for biofilm removal, offering practical implications for biofilm control in the food industry.

Keywords: Multidrug-resistant, *Staphylococcus aureus*, biofilm formation, stainless steel, disinfectants, elimination.

UTILIZATION OF NANOCELLULOSE-BASED NANOCOMPOSITES FROM PINEAPPLE LEAVES FOR SUSTAINABLE WASTEWATER TREATMENT IN AGRICULTURE

**Azima Azmi^{a*}, Mohammad Shahid Shahrin^b, Ainaa Abdul Kahar^a,
Muhammad Zaidi Abu Bakar^a & Shazwan Abd. Shukor^a**

^a*Biotechnology & Nanotechnology Research Centre, Malaysian Agricultural Research & Development Institute (MARDI), Persiaran MARDI-UPM, 43400 Serdang, Selangor.*

^b*Soil Science, Water & Fertilizer Research Centre, Malaysian Agricultural Research & Development Institute (MARDI), Persiaran MARDI-UPM, 43400 Serdang, Selangor.*

**Corresponding author: azima@mardi.gov.my*

Abstract

The increasing demand for sustainable agricultural practices necessitates the development of eco-friendly solutions for wastewater treatment. This study explores the use of nanocellulose-based nanocomposites derived from pineapple leaves as a potential material for wastewater treatment in agriculture. Pineapple leaves, an abundant agricultural waste, are rich in cellulose, making them an ideal source for nanocellulose extraction. By transforming these leaves into nanocellulose-based nanocomposites, this approach not only promotes waste valorization but also offers an environmentally friendly alternative to conventional wastewater treatment methods. The nanocomposites exhibit enhanced adsorption properties, which can effectively remove contaminants such as heavy metals, organic pollutants, and nutrients from agricultural wastewater. The high surface area and functional groups of nanocellulose enable strong interactions with pollutants, making it a promising material for water purification. Furthermore, the biodegradability and non-toxicity of nanocellulose ensure that these nanocomposites are safe for the environment and can be safely disposed of after use. This innovative application of pineapple leaf-derived nanocellulose in wastewater treatment presents a dual benefit: addressing agricultural waste management while improving water quality for sustainable farming. By incorporating these nanocomposites into agricultural practices, it is possible to reduce water pollution, promote resource efficiency, and enhance crop production through cleaner irrigation. Ultimately, this approach aligns with global efforts toward achieving sustainable agriculture, waste reduction, and environmental protection, contributing to the goals of clean water and responsible consumption in the context of agriculture.

Keywords: Pineapple, nanocellulose, nanocomposite, wastewater treatment



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INTRINSIC QUALITY OF STINGLESS BEE HONEYS OF SARAWAK

Margaret Abat^{a*}, Irna Syairina Sahari^a

^a*Agriculture Research Centre, Semongok, Department of Agriculture Sarawak
KM20, Borneo Heights Road, 93250 Kuching, Sarawak, Malaysia.*

^{*}*Corresponding author: margarea@sarawak.gov.my*

Abstract

Stingless bee or ‘*Kelulut*’ honeys are gaining an increasing demand owing to its unique characteristics than sweet honeys. In Sarawak, the industry is still at its infancy stage. Most of the past research works focused on the rearing and production of *kelulut* honeys. Information on the *kelulut* honey quality and downstream processing is rather limited^{1,2}. Furthermore, authenticity of the honey is of a major concern, which cannot be verified through visual examination or sensory tasting³. Currently, the only method to verify the authenticity of the honey is by doing a chemical analysis using a defined analytical equipment. The high quality and genuine *kelulut* honeys must meet the criteria set in the ‘Malaysian Standard MS 2683:2017 Kelulut (Stingless Bee) Honey - Specification’. In this work, compositional data of about 200 *kelulut* honeys sourced throughout Sarawak between 2017 and 2021 were compared with the Standard requirements. The samples were mostly non-processed or minimally processed honeys of the *Heterotrigona itama* and other *kelulut* species. The pH of *kelulut* honeys of Sarawak are between 1.52 and 3.82. The reducing sugar content of the samples are between 13.56 and 83.02 g/100 g, which is below the threshold level of 85 g/100 g. The concentration of total phenolic in the samples are between 14.50 and 321 mg GAE/kg, indicating the potential of anti-oxidant capacity of *kelulut* honeys. The minerals such as phosphorus, potassium, calcium, magnesium, iron and trace minerals are present at a considerable level in most samples. Only two samples contained hydroxymethylfurfural above the 30 mg/kg limit, an indication of a low quality honey. The results showed that the *kelulut* honeys of Sarawak are of good quality. Continuous monitoring of honeys’ quality by the relevant authority is critical to ensure the products in the markets meet the Standard requirements.

Keywords: *Kelulut*, honey, quality, minerals, antioxidant

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A DNA BIOSENSOR SYSTEM FOR DETECTING A BIOCIDES RESISTANT PEST (*T. mundella*) IN OIL PALM PLANTATIONS

Nurul Izzaty Hassan^{a,*}, Farah Asilah Azri^b, Lee Yook Heng^a, Gan Kok Beng^c, Aida Soraya Shamsuddin^d, Noorrezam Yusop^e, Mohamed Mazmira Mohd Masri^f & Mohd Rawa Ispal^b

^aDepartment of Chemical Sciences, Faculty of Science & Technology, UKM, 43600, Selangor, Malaysia

^bBiogenes Technologies Sdn Bhd, Jalan Maklumat, UPM, Serdang, Selangor

^cDepartment of Electrical, Electronic & Systems Engineering, Faculty of Engineering and Built Environment, UKM 43600, Selangor, Malaysia

^dInstitute for Environment and Development, Universiti Kebangsaan Malaysia (UKM), Bangi, 43600, Selangor, Malaysia;

^eFaculty of Information & Communication Technology, Technical University of Malaysia, Melaka(UTEM), Jalan Hang Tuah Jaya, 76100, Durian Tunggal, Melaka, Malaysia;

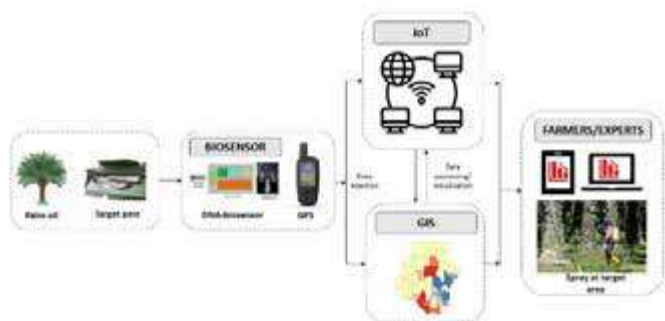
^fMalaysian Palm Oil Board(MPOB) Headquarters, Jalan Sekolah, Pekan Bangi Lama, 43000, Kajang, Selangor, Malaysia.

*Corresponding author: drizz@ukm.edu.my

Abstract

The development of resistance to pesticides in insects often involves genetic changes that alter the target site of the pesticide or enhance the insect's ability to detoxify or evade the pesticide. In animals, cadherin is a transmembrane protein that mediates cell-cell adhesion¹. The cadherin gene, which codes for cadherin proteins, can cause resistance to *Bacillus thuringiensis* (Bt), a commonly used biocide² in oil palm plantations to control the moth *Tirathaba mundella*. Therefore, a DNA biosensor has been developed to detect the resistance gene in the oil palm pest *T. mundella*. The electrochemical biosensor was used via transduction methods such as Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV). Larvae samples of *T. mundella* from an oil palm plantation in Sri Aman, Sarawak where infestation by Bt resistant *T. mundella* has been reported were collected and analyzed by using the DNA biosensor for cadherin genes to confirm the resistancy of the pest to the Bt biocide. The results obtained from the DNA biosensor indicated that the oil palms from the plantation were infected with *T. mundella* resistant to Bt, which was validated using PCR analysis. Additionally, a GIS-based system successfully mapped the estate over a four-year period, indicating potential resistance severity across different plantation zones. This spatial analysis aids in strategic intervention planning by pin-pointing high-risk areas requiring alternative pest control strategies as Bt may be no longer effective for pest control. This study has integrated smart technology for precision agriculture, enhancing decision-making in pest management. This holistic approach facilitates estate managers in effectively controlling and mitigating *T. mundella* resistance, ultimately improving crop yield and sustainability.

Keywords: *Tirathaba Mundella*, Cadherin gene, *Bacillus thuringiensis*, DNA biosensor, oil pam pest



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AN ELECTROCHEMICAL DETECTION OF FENVALERATE USING APTAMER WITH GRAPHENE-ACRYLATE COPOLYMER COMPOSITE MODIFIED ELECTRODE

Nurul Hidayah Ahmad Puat,^{a,b*} Sharina Abu Hanifah,^b Lee Yook Heng,^b Nur Azura Mohd Said,^a Suria Mohd Saad,^a Suhaina Supian,^a

^aMalaysian Agricultural Research and Development Institute, MARDI headquarters, Persiaran MARDI-UPM, 43400 Serdang, Selangor, Malaysia

^b Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia

*Corresponding author: p114694@siswa.ukm.edu.my

Abstract

This research investigates the detection of fenvalerate through an aptamer integrated with graphene-acrylate copolymer microspheres composites, enhancing conductivity and sensitivity for improved environmental monitoring and pesticide analysis. This study aims to develop an aptamer-based biosensor for fenvalerate detection. The synthesis of acrylate copolymer microspheres achieved via photo-polymerization and characterized using dynamic light scattering (DLS), field emission scanning electron microscopy (FESEM) and fourier transform infrared spectroscopy (FTIR) techniques. These microspheres composites were subsequently applied to carbon electrodes to serve as matrices for aptamer immobilization. The study also includes the electrochemical optimization of aptamer immobilization parameters such as type of electrolyte, pH, concentration, volume, incubation time, and temperature. A calibration curve for fenvalerate detection was constructed using EIS measurement with a 50 nM aptamer at 25 °C over 30 minutes. A linear calibration curve was obtained for fenvalerate concentration from 0 to 15 µM with regression value (R^2) of 0.9629. Furthermore, this biosensor achieved its limit of detection (LOD) of 773 nM. All measurements were conducted in a 0.1 M KCl solution at pH 7.0 with a 5 mM $[\text{Fe}(\text{CN})_6]^{3-/4-}$ (1:1 ratio). Percentage of recovery of fenvalerate in spiking samples using the liquid chromatography tandem mass spectrometry (LC-MS/MS) analysis was from 85 % to 112 % ($R^2 = 0.9976$), while using the biosensor method was from 96 % to 99 % ($R^2 = 0.9629$). These two methods showed a high correlation, refer to the regression value, $R^2 = 0.9827$. This indicates that the developed biosensor method has a high sensitivity and accuracy. In conclusion, this aptamer-based biosensor is a promising tool as an alternative method for detecting and monitoring fenvalerate residue in agricultural products and environments.

Keywords: Graphene; Polymer microspheres; Fenvalerate; Aptamer; Electrochemical biosensor

OILS EXTRACTED FROM INSECT BIOMASS FOR FOOD APPLICATIONS

L. C. Branco,* C. Esteves, K. Zalewska, M. J. Nunes, J. Lopes, A. F. M. Santos,
S. Freitas, A. Forte, A. V. Nunes

LAQV-REQUIMTE, Chemistry Department, NOVA School of Science and Technology,
NOVA University of Lisbon, 2829-516 Caparica, Portugal

*Corresponding author: l.branco@fct.unl.pt

Abstract

Food and Agriculture Organization of the United Nations (FAO) reported that approximately one in three people worldwide—equivalent to 2.37 billion individuals—lacked access to adequate food in 2020 [1]. This marked an alarming increase of nearly 320 million people in just one year [1]. Addressing this issue requires identifying sustainable and natural nutrient sources, such as insects [2]. Research in this field is expanding rapidly, and several companies in Portugal are dedicated to insect farming [3]. A new bioindustrial sector is emerging, bringing together academic and industrial partners to enhance the valorization of insect flour. This initiative aims to improve the extraction of oil and protein from insect biomass using sustainable green technologies [4]. In this study, the extraction of oil from *Tenebrio molitor* (mealworm) larvae flour was optimized. Solid-liquid extraction techniques were developed using green solvents, including task-specific ionic liquids and eutectic systems. The resulting extracts were analyzed using classical techniques such as Nuclear Magnetic Resonance Spectroscopy (NMR), Gas Chromatography-Mass Spectrometry (GC-MS), and Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS). The extraction yields were remarkably close to the expected total oil content in the insect flour. The extracted oils primarily contained triacylglycerols, which are an essential source of fatty acids.

Additionally, oil extractions were performed using flours derived from *Acheta domesticus* (domestic cricket) and *Hermetia illucens* (black soldier fly). The extracted oils and proteins from insect biomass show significant potential for applications in the food and cosmetic industries. This work is aligned with GOAL 2 ZERO HUNGER as Sustainable Goals from Agenda 2030.

Keywords: Food Products; Insect Flour Valorization; Proteins; Lipids; Sustainable extraction & purification

Acknowledgements

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ULTRA-SENSITIVE NANOTECHNOLOGY-ENABLED APTASENSOR FOR KANAMYCIN DETECTION IN DAIRY PRODUCTS

Rabti A.^{a,*}, Algethami F.K.^b, Ghodbane O.^a, Raouafi N.^c

^a National Institute for Research and Physicochemical Analysis (INRAP), Laboratory of Materials, Treatment, and Analysis (LMTA), Biotechpole Sidi Thabet, 2020 Sidi Thabet, Tunisia.

^b Department of Chemistry, College of Science, Imam Mohammad Ibn Saud Islamic University (IMSIU), P.O. Box 90950, Riyadh 11623, Saudi Arabia.

^c Sensors and Biosensors Group, Analytical Chemistry and Electrochemistry Lab (LR99ES15), University of Tunis El Manar, 2092 Tunis El Manar, Tunisia.

*Corresponding author: amal.rabti@fst.utm.tn

Abstract

This study presents a novel electrochemical aptasensor for the ultra-sensitive detection of kanamycin (KAN), an antibiotic widely used in veterinary medicine, which can pose significant health risks if present as residues in food products [1-2]. The aptasensor is based on a polyaniline/reduced graphene oxide (PANI/rGO) modified screen-printed carbon electrode (SPCE), leveraging the synergistic properties of PANI and rGO to enhance sensitivity and selectivity. By employing a dual-technique approach combining cyclic voltammetry (CV) and electrochemical capacitance spectroscopy (ECS), the sensor achieves a remarkable detection limit of $1.194 \text{ fg}\cdot\text{mL}^{-1}$ (CV) and $0.13 \text{ fg}\cdot\text{mL}^{-1}$ (ECS), with a dynamic range spanning from $1 \text{ fg}\cdot\text{mL}^{-1}$ to $1 \text{ ng}\cdot\text{mL}^{-1}$. The aptasensor's performance is attributed to the specific binding of KAN to the immobilized aptamer, which induces conformational changes that alter the electrode's electrochemical properties, particularly its specific capacitance. The ECS analysis further decomposes the capacitance response into double-layer and redox components, providing deeper insights into the interfacial changes and binding kinetics. The sensor's practical applicability was validated through successful detection of KAN in spiked milk samples, demonstrating recovery rates between 96% and 102%. This work highlights the potential of nanotechnology-enabled electrochemical sensors for sustainable agriculture, offering a highly sensitive, label-free, and cost-effective solution for monitoring antibiotic residues in food products, thereby contributing to food safety and environmental sustainability. The integration of advanced nanomaterials and electrochemical techniques paves the way for the development of next-generation biosensors for agricultural applications.

Keywords: Kanamycin Detection; Electrochemical Aptasensor; Polyaniline/Reduced Graphene Oxide; capacitance; Food Safety Monitoring.

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ASSESSMENT OF THE NUTRITIONAL CONTENT IN LOCALLY GROWN VEGETABLES AND THEIR SIGNIFICANCE IN PUBLIC HEALTH

Waziha Farha^{a, d*}, Md. Sayem Ali^b, Umme Habiba Rahman^c, Farhana Sobnom^d, Mohammad Shueb^d

^aDepartment of Textile Engineering, Bangladesh University of Business and Technology (BUBT),

Rupnagar, Mirpur-02, Dhaka, Bangladesh

^bDepartment of EEE, Bangladesh University of Business and Technology (BUBT), Rupnagar, Mirpur-02,

Dhaka, Bangladesh

^cDepartment of Economics, Bangladesh University of Business and Technology (BUBT), Rupnagar,

Mirpur-02, Dhaka, Bangladesh

^dDepartment of Chemistry, University of Dhaka, Dhaka-1000, Bangladesh

*Corresponding author: dfarha@bubt.edu.bd

Abstract

Local vegetables are cost-effective and culturally accepted sources of nutrition, making them crucial for addressing food security and malnutrition in developing regions supporting SDG 02 and 03 (*Zero hunger; Good health and well-being*). Some vegetables are hyper-accumulators of heavy metals and chain pathway (soil/environment – vegetable - human) of dietary exposure, which may pose health hazards to consumers of all ages. To study the effects of heavy metals on the nutritional values of vegetables, such as: pointed gourd (*Trichosanthes dioica*), bitter gourd (*Momordica charantia* L.), tomato (*Solanum lycopersicum* L.), chili (*Capsicum annum* L.) and cauliflower (*Brassica oleracea* var. botrytis) were collected from four different markets of Dhaka city and its peripheral areas. The concentrations of micronutrients for pointed gourd, bitter gourd, tomato, chili, and cauliflower, were found to be 26.14 - 50.03 mg/kg for Zn, 26.16-75.31 mg/kg for Fe, 11.83-34.59 mg/kg for Mn, 187.40-519.85 mg/kg for Ca and 3.95-12.77 mg/kg for Cu. Cadmium, Ni, and Pb were found in two vegetables, and Cr was observed only in bitter gourd. The minimal presence of heavy metals ensures the safe consumption of the studied vegetables, ensuring well-being (SDG 03). Promoting local vegetable farming and consumption can significantly improve public health by addressing malnutrition, reducing chronic diseases, and fostering food security while supporting sustainable local food systems.

Keywords: Vegetables, micronutrients, food security, sustainability, Public health.

APPLICATIONS OF ISOTOPE RATIO MASS SPECTROMETRY (IRMS) TO ORIGIN AND NATURALNESS CHARACTERISATION OF FOOD PRODUCTS

Lionnel Mounier

Thermo Fisher Scientific, 16 avenue du Québec SILIC 765 Villebon-sur-Yvette 91963 Coutaboeuf Cedex France

**Corresponding author: lionnel.mounier@thermofisher.com*

Abstract

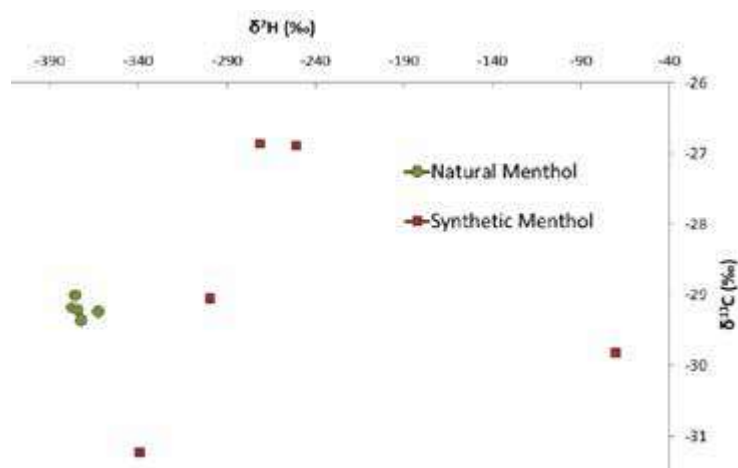
Several analytical methods, including chromatography, spectroscopy or mass spectrometry, can reveal adulterations or can enable to track the origin of food products. Isotope Ratio Mass Spectrometry (IRMS) is a particularly efficient technique when it becomes necessary to distinguish between the sources (what from) and between the origins (where from).

The isotope ratio fingerprinting is based on the analysis of small isotopic differences in compounds in order to determine the relative isotopic abundances of elements such as C, N, O, H and S contained in the material. The measured isotopic differences are originating from the physical and biochemical isotope fractionation occurring in nature, they are providing information about the source, the origin, and the naturalness of substances. Based on isotopic ratios it is possible to collect information about the geographical, the chemical or the botanical origin of substances. Isotopic ratios can enable the differentiation between natural and synthetic products.

The purpose of the presentation is to explore and to illustrate the state of the art in Isotope Ratio Mass Spectrometry used for characterization of the origin and the naturalness of food products.

Recent advances in instrumentation and in applications are highlighted.

Keywords: food authenticity, food adulteration, isotope fingerprinting, isotopic ratio mass spectrometry



Determination of the source of menthol by IRMS

SYNTHESIS OF ENVIRONMENTALLY SAFE PLANT RESISTANCE INDUCERS AS AN ALTERNATIVE TO PESTICIDES

Kukawka Rafal^{a,b,*}, Spychalski Maciej^{a,c}, Smiglak Marcin^a, Mikicinski Artur^c, Pulawska Joanna^c

^a Poznan Science and Technology Park, Adam Mickiewicz University Foundation, ul. Rubiez 46, 61-612 Poznan, Poland.

^b Innosil Sp. z o.o., ul. Rubiez 46, 61-612 Poznan, Poland

^c The National Institute of Horticultural Research, Konstytucji 3 Maja 1/3, 96-100 Skierniewice.

*Corresponding author: rafal.kukawka@ppnt.poznan.pl

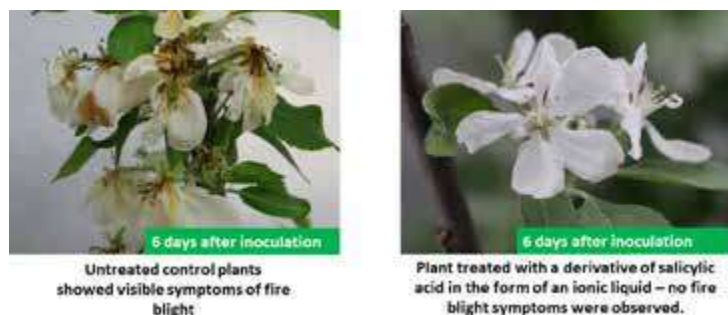
Abstract

The increasing global awareness of the environmental risks associated with pesticides has prompted the search for sustainable alternatives in plant protection. One promising strategy involves systemic acquired resistance (SAR) inducers—compounds that enhance plant immunity instead of directly targeting pathogens. Ionic liquids (ILs) are an emerging group of compounds offering a wide range of tunable physicochemical and biological properties, making them attractive candidates for agricultural use.

This study focused on the design, synthesis, and characterization of 45 novel ILs incorporating benzothiadiazole and salicylic acid derivatives—both recognized for their roles in activating plant defense responses. Structural variation was introduced through modifications of both cationic and anionic components, including biocompatible cations such as choline. All synthesized compounds were characterized by NMR spectroscopy, thermal analysis (DSC, TGA) and logP. Preliminary solubility and hydrolytic stability tests in aqueous media were conducted to assess their potential application in field conditions. A selected group of ILs was evaluated in vivo on apple trees for their ability to induce resistance against three major pathogens: (1) powdery mildew caused by *Podosphaera leucotricha*, (2) apple scab caused by *Venturia inaequalis*, and (3) fire blight caused by *Erwinia amylovora*. The results suggest that some of the tested ILs may act as effective SAR inducers and represent a promising direction for the development of next-generation, environmentally friendly crop protection agents.

The “Searching for new chemical compounds inducing resistance of apple to diseases and determination of the molecular mechanism of their action” project is carried out within the Sonata (UMO-2022/47/D/NZ9/02327) programme of the National Science Center, Poland

Keywords: ionic liquid, systemic resistance inducers, salicylic acid, benzothiadiazole



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UNLOCKING THE FUTURE OF FOOD: ELEMENTAL INSIGHTS INTO ALTERNATIVE PROTEINS WITH ORGANIC ELEMENTAL ANALYSIS

Cheah Chris*, Patel Dhaval

Thermo Fisher Scientific, 1 Science Park Road, Singapore Science Park 2, Singapore 117528

**Corresponding author: chris.cheah@thermofisher.com*

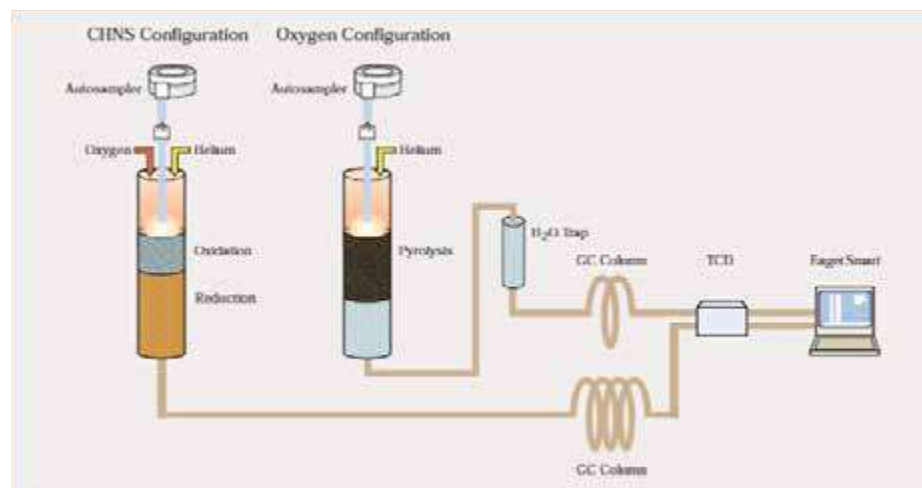
Abstract

As global demand for sustainable and nutritious food sources grows, alternative proteins—derived from plants, insects, fungi, and cultured cells—are emerging as vital solutions to address environmental, ethical, and health concerns. However, ensuring the nutritional quality, consistency, and safety of these novel proteins requires robust analytical tools.

Organic elemental analyzers offer rapid and accurate quantification of key elements - carbon (C), hydrogen (H), nitrogen (N), and sulfur (S), which are essential for determining protein content, purity, and nutritional value. Unlike conventional methods, organic elemental analyzer platform provides automated, high-throughput analysis with minimal sample preparation, making it ideal for research, quality control and production environments.

Through a series of real-world case studies, the presentation will explore the application of elemental analysis in evaluating a diverse range of alternative proteins, including plant-based meat analogues, microalgae, and insect-derived products. Emphasis will be placed on nitrogen-to-protein conversion, batch consistency assessment, and the detection of adulteration or contamination. By integrating elemental analysis into the R&D and manufacturing pipeline, the food industry can ensure transparency, traceability, and nutritional excellence in the alternative protein space.

Keywords: alternative protein, nutritional quality, future food, plant-based meat, organic elemental analyzer, food adulteration, food quality



LC-MS MOLECULAR NETWORKING AND MULTIVARIATE ANALYSIS REVEAL ANTIOXIDANT CONSTITUENTS IN THE MALAYSIAN CULINARY HERB KESUM (*POLYGONUM MINUS HUD.*)

Adiez Sapura Azmi^a, Shahida Muhamad Mukhtar^b, Fatimah Salim^{a,c,*}

^aFaculty of Applied Sciences, Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia.

^bFaculty Pharmacy, Universiti Teknologi MARA Selangor Branch, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor, Malaysia.

^cAtta-ur-Rahman Institute for Natural Product Discovery (AuRIns),

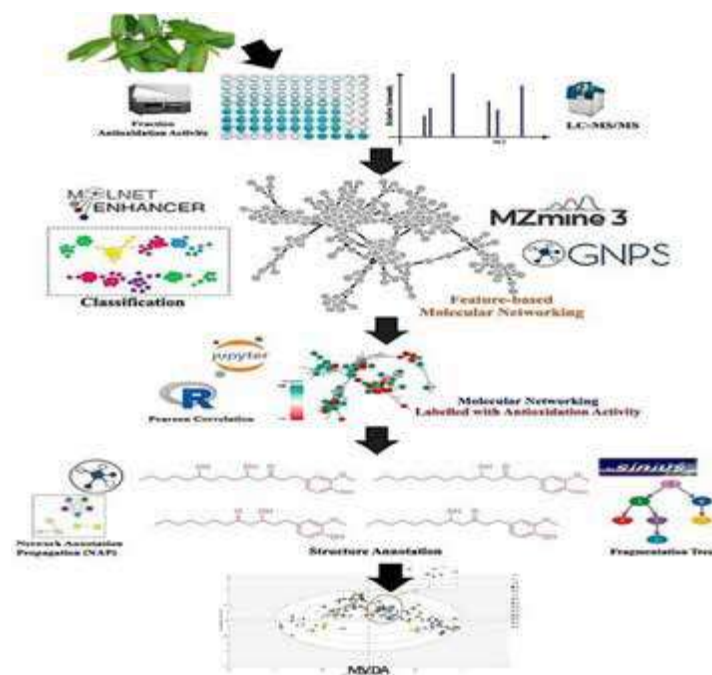
Universiti Teknologi MARA Selangor Branch, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor, Malaysia.

*Corresponding author: fatimah2940@uitm.edu.my

Abstract

Kesum (*Polygonum minus* Hud.) is a traditional aromatic herb widely used in Malaysian culinary practices and is recognized for its strong antioxidant activity, attributed to its rich flavonoid and phenolic content. This study aimed to evaluate the antioxidant potential of both ethanolic crude and clean-up extracts of Kesum using DPPH, ABTS, and FRAP assays. The clean-up extract demonstrated better antioxidant activity, with IC₅₀ values of 194.03 ± 8.09 µg/mL (DPPH) and 141.03 ± 4.81 µg/mL (ABTS), and a FRAP value of 14,478.99 ± 7.93 µmol AAE/mg extract. To further explore the phytochemical differences between the extracts, tandem liquid chromatography–mass spectrometry (LC-MS) molecular networking coupled with multivariate data analysis (MVDA) was employed. Eight major clusters of phytochemicals were identified, predominantly comprising flavonols and their derivatives (isoquercetin, hyperoside, quercetin 3-O-glucuronide, quercitrin, kaempferol 3-glucuronide, astragalin, and trifolin), flavones (isoscutellarin, scutellarin, and 6-hydroxyluteolin), and sesquiterpenoids (americanolide D, 4H-tomentosin, and lactarorufin A). These compounds were reported for the first time in the clean-up Kesum extract. PLS-DA modeling revealed that the DPPH scavenging activity was primarily associated with quercetin 3-O-glucuronide, luteolin 7-sulfate, and robinetin, whereas ABTS and FRAP activities were correlated with ayanin and isopetasol, and euphodendriane A and cucurbitacin B, respectively. The clean-up extract of Kesum exhibited enhanced antioxidant properties and a richer profile of bioactive compounds compared to the crude extract. The identification of novel flavonoids and sesquiterpenoids highlights Kesum's potential as a functional food or nutraceutical ingredient. Further studies are recommended to isolate and characterize the individual bioactive compounds to better understand their specific antioxidant mechanisms. Additionally, in vivo antioxidant assays should be conducted to support potential therapeutic applications and commercial development of Kesum-based products.

Keywords: antioxidant, flavonoids, molecular networking, LC-MS, MVDA



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EFFECT OF SUPERCRITICAL FLUID TEMPERATURE ON THE PHYSICOCHEMICAL PROPERTIES OF SACHA INCHI (*Plukenetia volubilis*) SEED OIL

Siti, R.^{a*} and Mohd Hazwan, A.H^a

^a*Universiti Teknologi MARA*

*Corresponding author: sitis009@uitm.edu.my

Abstract

Sacha inchi (SI) also known as *Plukenetia volubilis* seed oil is renowned for its health benefits, typically extracted via cold pressing, which yields only partial oil recovery. Conventional methods like hexane extraction pose risks of oil deterioration and involve toxic, flammable solvents. This study aims to extract SI seed oil using Supercritical Fluid Extraction (SC-CO₂) at varying temperatures (30°C, 40°C, 50°C, 60°C) and evaluate its physicochemical properties. Oil yield increased with temperature (19.96% at 30°C to 32.11% at 60°C). Higher temperatures reduced melting point (6.50 to 4.00) and smoke point (236.50 to 164.00), indicating thermal sensitivity. However, oxidation stability declined at higher temperatures, with iodine value (IV) 187.42 to 204.50 and peroxide value (PV) 3.50 to 34.50 rising significantly. The optimal extraction temperature was 60°C for maximising yield and maintaining functional properties (melting/smoke points), but 30°C was superior for oxidative stability. The findings highlight a trade-off between yield and stability in SC-CO₂ extraction of SI oil. This research provides a practical method to extract high-quality Sacha inchi oil safely and efficiently, supporting Malaysia's goals for healthier food production and sustainable industrial development.

Keywords: Sacha inchi oil, Supercritical fluid extraction (SC-CO₂), Oxidative stability, Physicochemical properties, Sustainable extraction

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FUTURE FOOD: VALUABLE COMPOSITION OF INDIAN BORAGE LEAVES (*PLECTRANTHUS AMBOINICUS*) AND NEEM LEAVES (*AZADIRACTHA INDICA*) USING SOLVENT EXTRACTION

Khairunnisa Yusra Abdul Rahman¹, Aida F. M. N. A¹, Razif Dasiman², Nazimah Hamid³
and Siva Raseetha¹

¹Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia

²Faculty of Health Sciences, Universiti Teknologi MARA Selangor, 42300 Puncak Alam, Selangor, Malaysia

³Department of Food Science and Microbiology, Auckland University of Technology, New Zealand

*Corresponding author email: raseetha@uitm.edu.my

Abstract

This research investigates the physicochemical characterisation of bioactive compounds extracted from the leaves of Indian borage (*Plectranthus amboinicus*) and neem (*Azadirachta indica*) using solvent extraction with 50% and 95% ethanol. The study addresses the limited availability of sustainable and efficient extraction methods for bioactive compounds. The research aims to assess antioxidant activity, antimicrobial properties, and physicochemical characteristics including colour, chlorophyll, functional groups and volatile compounds. Ethanol extracts were analysed for colour using a Chromameter CR-400, antioxidant potential via DPPH assay, functional groups with Fourier-transform infrared spectroscopy (FT-IR) and volatile compounds using gas chromatography-mass spectrometry (GC-MS). Chlorophyll content including chlorophyll-a, chlorophyll-b and total chlorophyll was quantified using spectrophotometric method. Results revealed that 50% ethanol extracts exhibited DPPH radical scavenging activity between 87% to 89% due to the effective extraction of hydrophilic antioxidants, while 95% ethanol extracts demonstrated stronger antimicrobial activity against common foodborne pathogens with inhibition zones ranging from 1.06 cm to 1.52 cm, attributed to the extraction of hydrophobic bioactive compounds. This study highlights the influence of solvent polarity and processing methods on the bioactive properties of *P. amboinicus* and *A. indica*, emphasising their potential as sustainable sources of antioxidants and antimicrobials for applications in food, pharmaceuticals, and cosmetic products.

Keywords: *Plectranthus amboinicus*, *Azadirachta indica*, bioactive compounds, antioxidant activity, antimicrobial properties



Indian borage (*Plectranthus amboinicus*)



Neem (*Azadirachta indica*)

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BRIDGING TRADITION AND SCIENCE: IMPROVING INDIGENOUS MEDICINE IN SRI LANKA

Paranagama P. A.^{a *}

Department of Chemistry, University of Kelaniya, Sri Lanka

*Corresponding author: priyani@kln.ac.lk

Abstract

Indigenous medicine has long been a cornerstone of healthcare systems worldwide, particularly in regions with rich ethnomedical traditions. The use of herbal formulations rooted in Ayurveda, Unani, Siddha and traditional medical systems. Traditional knowledge has demonstrated remarkable potential for treating a wide range of ailments. However, the integration of these practices into modern healthcare systems necessitates enhancements in product quality and bioactivity to ensure efficacy, safety, and reproducibility. There are many studies focusing on developing systematic approaches to improve the quality and bioactivity of indigenous medicinal products, with an emphasis on standardization, scientific validation, and advanced formulation techniques. Key objectives include the identification of active compounds in underutilized medicinal plants, optimization of extraction methods to maximize bioactive yields, and the application of quality control measures such as chromatographic profiling and spectroscopic analysis. The role of cutting-edge technologies, such as nanotechnology and targeted delivery systems, is also explored to enhance the bioavailability and therapeutic potential of herbal medicines. Additionally, the research highlights the importance of preserving the traditional knowledge associated with indigenous medicine while incorporating modern scientific methodologies. Efforts to ensure sustainable sourcing of raw materials, minimize batch-to-batch variability, and comply with global regulatory standards are also emphasized. Case studies involving polyherbal formulations are presented to demonstrate improved antioxidant, anti-inflammatory, and antidiabetic activities through process optimization. By bridging the gap between traditional wisdom and contemporary science, this study aims to elevate the global acceptance of indigenous medicine as a reliable and effective healthcare alternative. Enhancing product quality and bioactivity not only reinforces consumer confidence but also contributes to the economic empowerment of local communities engaged in the cultivation and processing of medicinal plants. The findings highlight the potential for indigenous medicine to play a pivotal role in addressing current and emerging health challenges globally.

Keywords: Indigenous medicine, Ayurveda, Unani, medicinal plants

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IMMUNOSUPPRESSIVE AND ANTI-INFLAMMATORY ACTIVITIES OF NATURAL α,β -UNSATURATED CARBONYL-BASED COMPOUNDS ON THE IMMUNE SYSTEM

Ibrahim Jantan

Institute of Systems Biology (INBIOSIS), Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia

**Corresponding author: profibj@gmail.com*

Abstract

α,β -Unsaturated carbonyl-based compounds are considered to be the reactive substructures of natural products, hence, owing miscellaneous pharmacological activities i.e., potent antioxidant, antiinflammatory, antiviral, antibacterial, antifungal, antitubercular, and immunomodulatory properties. The most important and widely studied α,β -unsaturated carbonyl-based compounds include the natural products, curcumin, chalcones, zerumbone and their analogs and derivatives. We synthesized different novel series of α,β -unsaturated carbonyl-based compounds and they were investigated for various *in vitro* and *in vivo* activities.

The findings encouraged us to evaluate the effects of natural α,β -unsaturated carbonyl-based compounds on the innate and adaptive immune systems and hence explored the relationship between the inhibitory effects and chemical structures of the compounds. The compounds were investigated for their effects on phagocytosis process, specific actions on immune cells, effector mechanisms, nitric oxide (NO) and reactive species productions, and signaling pathways in human neutrophils, monocytes and macrophages. The samples were also assessed for their *in vivo* modulatory effects on the humoral and cellular immune functions both in innate and adaptive immune responses in rats and mice. The findings indicate that α,β -unsaturated carbonyl-based compounds effectively inhibited the innate and adaptive immune responses in immune cells and animal models. Their anti-inflammatory activities were partially mediated by their suppressive effects on pro-inflammatory cytokines expression, prostaglandin, COX-2 and NO production via NF- κ B, MAPKs and PI3K-Akt signaling pathways. α,β -Unsaturated carbonyl-based compounds may serve as leads for development into potent immunomodulating agent in treating different immune related diseases particularly related to inflammatory disorders.

Keywords: α,β -unsaturated carbonyl-based compounds, immune systems, anti-inflammatory, immunosuppression.

DEVELOPMENT OF BETTER BEDAQUILINE FOR MULTI-DRUG-RESISTANT TUBERCULOSIS

Peter J. Choi^{a*}, Hamish S. Sutherland^a, Brian D. Palmer^a, William A. Denny^a and Christopher B. Cooper^b

^a*University of Auckland*

^b*TB Alliance*

**Corresponding author: p.choi@auckland.ac.nz*

Abstract

Bedaquiline is a novel drug approved in 2012 by the FDA for the treatment of drug-resistant tuberculosis (TB). Although it shows high efficacy towards drug-resistant forms of TB, its use has been limited by the potential for significant side effects. In particular, bedaquiline is a very lipophilic compound with an associated long terminal half-life. It shows potent inhibition of the cardiac potassium hERG channel, resulting in QTc interval prolongation in humans and possibly cardiac arrhythmia. To address these issues, we carried out a drug discovery program to develop improved second-generation analogues of bedaquiline. This drug discovery program identified two lead candidates, TBAJ-576 and TBAJ-876, which are currently undergoing human clinical trials. This talk will highlight the medicinal chemistry efforts in synthesizing the improved analogues, metabolite identification, and future directions for further improving the bedaquiline analogues.

Keywords: bedaquiline; TBAJ-876; TBAJ-576; mycobacterium tuberculosis; drug development

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PROTEASOME INHIBITOR: SYNTHESIS, EVALUATION AND MOLECULAR SIMULATION

Khor Poh-Yen,^{a*} Lam Kok-Wai,^b Johnson Stanslas,^c Mock Phooi-Yan,^b Heng Kai Yen^d

^a*Universiti Kuala Lumpur, Royal College of Medicine Perak, Faculty of Pharmacy and Health Sciences*

^b*Universiti Kebangsaan Malaysia, Faculty of Pharmacy*

^c*Universiti Putra Malaysia, Faculty of Medicine and Health Sciences*

^d*Biomed Global (M) Sdn. Bhd.*

**Corresponding author: pykhor@unikl.edu.my*

Abstract

Inhibit proteasome degradation activity has been suggested as a promising treatment strategy for cancer.¹ Existing approved proteasome inhibitors are challenged with low anti-cancer effects on solid tumours and severe side effects,² necessitating the exploration of new potential proteasome inhibitors. We have been using a greener drug discovery approach: ultrasonic-mediated aldol-condensation synthesis and molecular simulation to discover a selective small molecule to target triple-negative breast cancer (TNBC). The Structure-Activity-Relationship (SAR) and cell proliferation assays identified a lead compound that selectively inhibits TNBC cell proliferation (SI > 10) at 380 nM. Further *in vitro* bioactivity and molecular simulation analysis show that lead is a small molecule that

- Inhibit proteasome degradation activity
- Stabilized pro-oncogenic proteins via the ubiquitin-proteasome pathway
- Induce apoptosis cell death
- Arrest cell cycle progression
- Attenuate cell migration

As a result, ultrasonic-mediated synthesis and molecular simulations have successfully discovered proteasome inhibitors targeting triple-negative cancer.

Keywords: synthesis, proteasome, inhibitor, docking

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NEW FAMILY OF POLY(AMIDOAMINE) DENDRIMERS AND DENDRONS FOR MAGNETIC RESONANCE IMAGING (MRI) APPLICATION

Saïd El Kazzouli*

Euromed University of Fes, 30000 Fez, Morocco

**Corresponding author: s.elkazzouli@ueuromed.org*

Abstract

Nowadays, there is a very strong demand for versatile agents suitable for non-invasive magnetic and/or optical imaging in living organisms¹. In this communication, we will present the design and synthesis of new families of dendrimers and dendrons that take advantage of the unique structure of dendrimers^{1,2}. Using the poly-(amidoamine) (PAMAM) dendrimer structure, we wish to promote the biocompatibility of the system and to have functional groups available at the surface to obtain specific functionalities such as the ability to coordinate nanoparticles such as magnetic iron oxides. So, a divergent synthesis and characterization by NMR and mass spectrometry of PAMAM dendrimers and dendrons will be presented. The result of biological and magnetic properties of the magnetic iron oxide dendrimers and magnetic iron oxide dendrons will be discussed. We believe that our results represent a promising approach for the design of a biocompatible magnetic iron oxide nanoparticles as versatile MRI agents.

Keywords: Dendrimers, Dendrons, Magnetic resonance imaging (MRI), Iron oxides, PAMAM

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NMR-BASED STABILITY EVALUATION OF (*E*)-1-(3',4'-DIMETHOXYPHENYL)BUTADIENE FROM *ZINGIBER CASSUMUNAR* ROXB. RHIZOME

**Chatkamon Lekwongphaiboon^a, Boonwiset Seaho^a, Wichayasith Inthakusol^{b,c},
Saisuree Prateptongkum^a, Wacharee Harnying^d, Albrecht Berkessel^d, and
Nongnaphat Duangdee^{b,c,*}**

^a*Department of Chemistry, Faculty of Science and Technology,
Thammasat University (Rangsit Campus), Pathum Thani, Thailand*

^b*Drug Discovery and Development Center, Office of Advanced Science and Technology,
Thammasat University (Rangsit Campus), Pathum Thani, Thailand*

^c*Thammasat University Research Unit in Cannabis and Herbal Products Innovation,
Thammasat University (Rangsit Campus), Pathum Thani, Thailand*

^d*Department of Chemistry (Organic Chemistry), University of Cologne, Cologne, Germany*

^{*}*Corresponding author: nongnaphat.duangdee@gmail.com*

Abstract

(*E*)-1-(3',4'-dimethoxyphenyl) butadiene (DMPBD) is a phenylbutanoid phytochemical found in *Zingiber cassumunar* Roxb. It is an anti-inflammatory compound with the potential as a candidate drug. However, its instability limits its potential for pharmaceutical applications. In drug development, the stability of active compounds must be assessed to ensure they retain their properties from production to application. Therefore, improving the stability of DMPBD is crucial for maintaining its efficacy. This study investigates the factors affecting the stability of DMPBD under various conditions including different solvents, temperatures, storage conditions, and light exposure over one month. Quantitative ¹H NMR (qNMR) with an internal standard was used to monitor the amount of DMPBD retained, optimize storage conditions, and identify key factors influencing its stability. The optimized storage conditions for preserving DMPBD involve using methanol-*d*₄ as a solvent and storing it below 4°C to maintain its integrity in both methanolic and crude extracts. Exposure to light has a minor adverse impact, leading to a reduction in DMPBD content. Additionally, storage in chloroform-*d* results in the decomposition of DMPBD, and some degradation occurs via O₂-induced cleavage of the diene moiety.

In conclusion, DMPBD in a purified compound and crude extract forms should be stored in methanol-*d*₄ below 4°C and protected from oxygen to prevent degradation. These optimized storage conditions are essential for maintaining stability in pharmaceutical and research applications.

Keywords: DMPBD, qNMR, stability evaluation, *Z. Cassumunar*

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STUDY OF ANTI OBESITY EFFECT THROUGH INHIBITION OF PANCREATIC LIPASE ACTIVITY OF *TRADESCANTIA SPATHACEA* LEAVES

Win-Nie Ng^a, Khye-Er Loh^b, Sook-Yee Liew^{c, d}, Siow-Ping Tan^{a, *}

^a Department of Physical Science, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Kuala Lumpur 53300, Malaysia.

^b Department of Bioscience, Faculty of Applied Sciences, Tunku Abdul Rahman University of Management and Technology, Kuala Lumpur 53300, Malaysia

^c Chemistry Division, Centre for Foundation Studies in Science, Universiti Malaya, Kuala Lumpur, Malaysia.d

^d Centre for Natural Products Research and Drug Discovery (CENAR), Universiti Malaya, Kuala Lumpur, Malaysia.

*Corresponding author: tansp@taru.edu.my

Abstract

Obesity is the most prevalent global metabolic disorder which contributes to various health risks that impact society worldwide. Although synthetic anti-obesity drugs exist, they frequently give adverse side effects, prompting a growing interest in natural products as safer and more effective alternatives. To the best of our knowledge, no studies have been reported on the anti-obesity effects of *Tradescantia spathacea* leaves. The aim of this study is to evaluate the pancreatic lipase (PL) inhibitory effects of *Tradescantia spathacea* leaves. Orlistat will be used as positive control. Ultrasonic-assisted extraction, solvent partitioning and fractionation techniques will be used to obtain hexane, dichloromethane and ethyl acetate crude extracts and their subfractions. The extracts and subfractions will then be analyzed for PL inhibitory activity. The results showed that the dichloromethane crude extract exhibited the highest PL inhibition rate of 97.73±0.59%, followed by ethyl acetate crude extract (90.89±0.05%) and hexane crude extract (43.80±1.80%) at 10 mg/mL. Dichloromethane and ethyl acetate extract were chosen to be further isolated into their respective fractions. There are three dichloromethane subfractions and four ethyl acetate subfractions showed PL inhibition rate more than 60%. Three dichloromethane subfractions exhibited IC₅₀ value of 1.57±0.06, 1.78±0.01 and 2.16±0.08 mg/mL while four ethyl acetate fractions exhibited IC₅₀ value of 0.53±0.03, 1.30±0.11, 1.10±0.12 and 2.37±0.27 mg/mL, respectively. The results of this study suggest that *T. spathacea* has great potential as a valuable source against obesity and is amenable to further purification processes to isolate their bioactive components that contribute to the PL inhibitory effects.

Keywords: Commelinaceae; *Tradescantia spathacea*; antiobesity; pancreatic lipase inhibition; Ultrasonic-assisted extraction.

BIFLAVONOIDS FROM *Araucaria* AS A POTENTIAL PDE4 INHIBITORS: IN SILICO AND IN VITRO STUDIES

Nafisah^a, Purwantiningsih Sugita^{a,*}, Budi Arifin^b, Setyanto Tri Wahyudi^b, Uus Saepuloh^c, Silmi Mariya^c

^aDepartment of Chemistry, IPB University, Indonesia.

^bDepartment of Physics, IPB University, Indonesia.

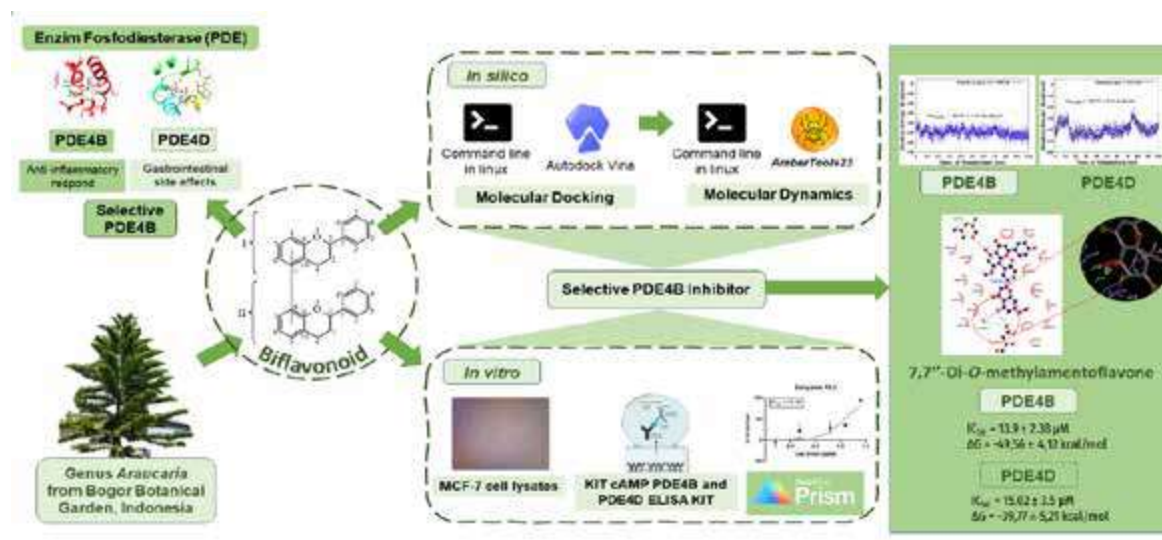
^cPrimate Research Centre, IPB University, Indonesia.

*Corresponding author: purwantiningsih@apps.ipb.ac.id

Abstract

Phosphodiesterase-4 (PDE4), particularly the PDE4B isoform, plays a key role in inflammatory regulation and is a promising target for anti-inflammatory therapy. The genus *Araucaria* is known to be rich in biflavonoids, a class of compounds with diverse biological activities, including anti-inflammatory effects.¹ This study evaluates the anti-inflammatory potential of biflavonoids from *Araucaria* through in silico and in vitro approaches, focusing on PDE4B and PDE4D inhibition. Molecular docking of 25 biflavonoid compounds was performed using AutoDock Vina against PDE4B and PDE4D. The selected complexes underwent molecular dynamics simulations with AMBER22, including six biflavonoid isolates from *Araucaria hunsteinii* and *Araucaria cunninghamii* leaves from Bogor Botanical Garden, Indonesia, that had been isolated previously.^{2,3} The in vitro activity of six selected isolates was tested using the ELISA method with MCF-7 cell lysates. The results identified 7,7''-di-*O*-methylenflavone as a selective PDE4B inhibitor, with an IC₅₀ value of 13.9 ± 2.38 µM. This compound exhibited strong binding affinity, favorable MM/GBSA binding energy, and high stability during molecular simulations, highlighting its potential as a promising candidate for anti-inflammatory drug development.

Keywords: Biflavonoid, ELISA, molecular docking, molecular dynamics, PDE4 inhibitor



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NOVEL HYBRID MOLECULES FROM 2-AMINO-4-ARYL THIAZOLE AND 2-METHYL-5-NITRO-3-PHENACYL NITROIMIDAZOLE AS AN ALTERNATIVE FOR LEISHMANIASIS AND TRYPANOSOMIASIS CAUSED BY *L. MEXICANA* AND *T. CRUZI*

MSc. Ramirez-Sandoval Cristoper ^a* & Dr. Campos-Aldrete Maria-Elena ^a*

^a Escuela Nacional De Ciencias Biológicas. Instituto Politécnico Nacional. México City, México.

*Corresponding author: christunning1@gmail.com, comesol22@gmail.com

Abstract

According to the WHO [1], at least about thirty percent of the population has experienced one or more parasitic events. Parasitic diseases caused by vectors is another branch of diseases that have been taken as forgotten or neglected by migratory, political and socioeconomic phenomena, but today they have already become global and of medical relevance, an example of this is leishmaniasis and trypanosomiasis caused by *L. mexicana* and *T. cruzi*. These vector-borne parasitosis afflict large vulnerable sectors of the population, despite the fact that there is treatment available on the market, they possess disadvantages on the effectiveness and toxicity, therefore, the use of 2-amino-4-aryl thiazoles and 3-phenacyl-2-methyl-5-nitroimidazole as scaffolds to build novel hybrid heterocyclic systems to treat the parasitosis caused by the aforementioned vectors will be of great relevance in this study.

A screening of different candidate molecules for the synthesis of hybrid compounds was carried out, using bioinformatical tools to build a molecular coupling analysis, the possible affinity and inhibition potential of each of the molecules against two types of oxidoreductases involved in the metabolism of the etiological agents, such as Thioredoxin reductase (PDB: 4CBQ) [2] and Trypanothione reductase (PDB: 1BZL) [3]. To determine the biological activity in the leishmaniasis model, a multipanel assay was performed with two variables: concentration and structural variation, using a vital dye (blue alamar) to determine the MIC and IC₅₀ using fluorescence and/or absorbance. On the other hand, to determine trypanomicidal activity, a test was carried out based on the methodology proposed by Pizzi-Brenner to determine IC₅₀.

Based on the method presented above, the series of hybrid compounds present a better antiparasitic potential in both etiological agents compared to the reference drugs, exposing the structural chemical contribution in each of the nuclei, demonstrating the electronic potential due to the high conjugation of the molecule, therefore the increase in antiparasitic activity with the sum of each of the specific groups inserted in the final molecules.

Keywords: Thiazole, Imidazole, *Leishmania mexicana*, *Trypanosoma cruzi*, Medicinal chemistry.

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CYTOTOXIC PROPERTIES OF BIFLAVONOIDS FROM INDONESIAN *ARAUCARIA*: A POTENTIAL LEAD FOR ANTICANCER THERAPY

Purwantiningsih Sugita^{a,*}, Dhea Demitri Agusta^a, Kurniawanti^a, Luthfan Irfana^a, Hanhan Dianhar^b, Irma Herawati Suparto^a, Dyah Utami Cahyaning Rahayu^c

^aDepartment of Chemistry, Faculty of Mathematics and Natural Sciences, IPB University, Bogor, West Java, Indonesia

^bChemistry Study Program, Faculty of Mathematics and Natural Sciences Universitas Negeri Jakarta, Jakarta, Indonesia

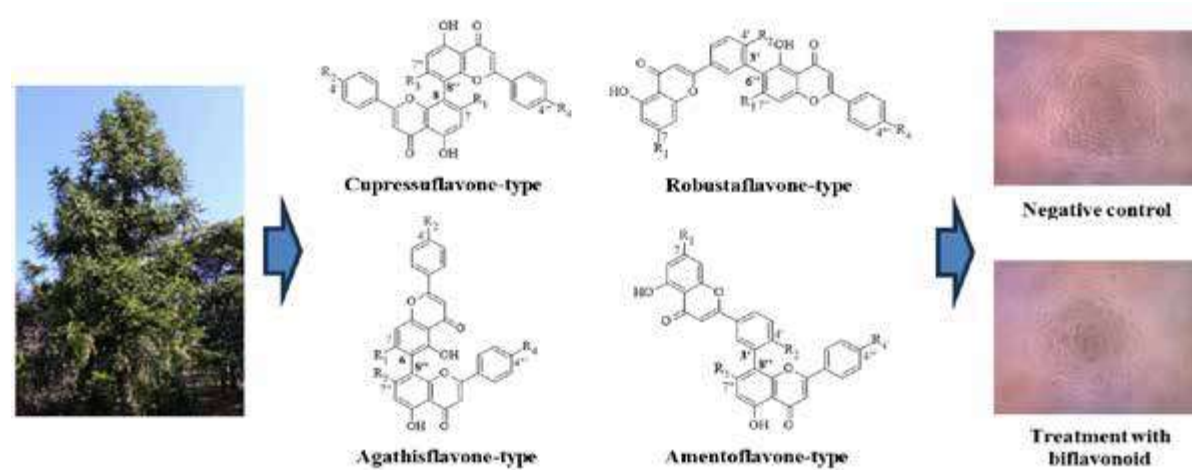
^cDepartment of Chemistry, Faculty Mathematics and Natural Sciences, Universitas Indonesia, Depok, West Java, Indonesia

*Corresponding author: purwantiningsih@apps.ipb.ac.id

Abstract

Biflavonoids are phenolic compounds formed by the oxidative coupling of two flavonoid units, exhibiting anticancer activity. Despite various therapies and preventive efforts, natural herbal medicine remains a safer and more affordable alternative for treatment. This study aims to isolate biflavonoids from selected *Araucaria* plants and conduct several anticancer tests. Nine biflavonoids classified in agathisflavone-, amentoflavone-, cupressuflavone-, and robustaflavone-type were successfully isolated from *A. hunsteinii*,¹⁻² *A. columnaris*,³ and *A. cunninghamii*.⁴ Herein, the discussion will be focused on anticancer activities of all compounds against MCF-7 (human breast), HeLa (immortal human), and calf pulmonary arterial endothelial (CPAE) cancer cells using MTT assay. In this study, we successfully identified one amentoflavone- and two cupressuflavones-type of biflavonoids that show potential as lead anticancer agents with IC₅₀ ranging from 1.4 ± 1.1 (strong inhibitory) to 99.2 ± 1.4 μM (weak inhibitory).¹⁻³ The structure-activity relationship of biflavonoids will also be discussed.

Keywords: anticancer, *Araucaria*, biflavonoids, cytotoxic



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IN-SILICO PREDICTION OF BIFLAVONOIDS FROM INDONESIAN *ARAUCARIA CUNNINGHAMII* MUDIE AS NON-COVALENT PROTEASOME INHIBITORS

Luthfan Irfana^{a,*}, Budi Arifin^a, Setyanto Tri Wahyudi^b, Suminar Setiati Achmadi^a,
Purwantiningsih Sugita^a

^aDepartment of Chemistry, Faculty of Mathematics and Natural Sciences, IPB University, Indonesia

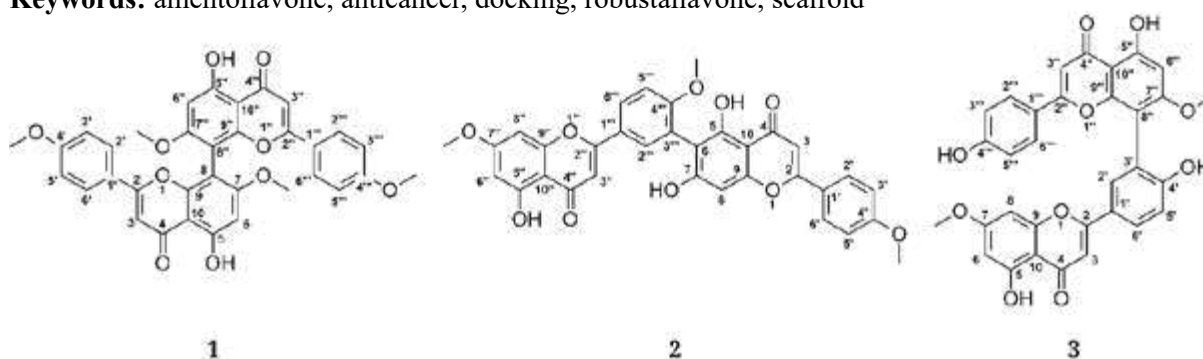
^bDepartment of Physics, Faculty of Mathematics and Natural Sciences, IPB University, Indonesia.

*Corresponding author: luthfan.irfana@apps.ipb.ac.id

Abstract

The *Araucaria* genus is rich in biflavonoid content. The latest theory suggests the anticancer activity of several biflavonoids might stem from the inhibition of the 20S proteasome. Although proteasome is an important target in cancer research, the development of its inhibitors is too focused on the reactive warhead-bearing covalent type. There is a growing need for new non-covalent inhibitor natural products-inspired scaffolds which are generally safer. Three biflavonoid compounds have been isolated from the leaves of Indonesian *Araucaria cunninghamii* Mudie in our previous research¹. *In-vitro* treatment with 7,7''-di-*O*-methylamentoflavone (**3**) caused the best cytotoxicity and the steepest decrease of proteasome concentration in the MCF7 cell line, followed by 7,4',7'',4'''-tetra-*O*-methylcupressuflavone (**1**), and 4'''-tri-*O*-methylrobustaflavone (**2**). Here we use molecular docking, molecular dynamics, and 3D-QSAR partial least squares (PLS) regression model to predict the probability of these compounds to inhibit proteasome chymotrypsin-like activity non-covalently. Molecular docking and 100 ns molecular dynamics predicted all compounds to have favorable binding free energy with $\beta 5$ subunit. Compound **3** ($\Delta G_{\text{GBSA}} = -23.9$ kJ/mol) have the best chance to form stable hydrogen bond with the vital THR1 residue (14% occupancy). Meanwhile, compounds **2** ($\Delta G_{\text{GBSA}} = -26.4$ kJ/mol) and **1** ($\Delta G_{\text{GBSA}} = -42.9$ kJ/mol) are likely interact more hydrophobically with the target. Furthermore, we have trained a 3D-QSAR PLS model (PC = 5, $r^2 = 0.9607$, $q^2_{\text{LOO}} = 0.6418$, SDEC = 0.1929, SDEP = 0.5823) using non-covalent $\beta 5$ inhibitor assay data manually curated from ChEMBL ($n = 76$, $p\text{IC}_{50 \text{ min}} = 5.2$, $p\text{IC}_{50 \text{ max}} = 8.9$). The predicted $p\text{IC}_{50}$ values are 8.67 (**3**), 8.19 (**2**), and 6.75 (**1**). These results suggest that the amentoflavone and robustaflavone scaffold might be more potent than the cupressuflavone in inhibiting the proteasome activity, thus more worthy for future development.

Keywords: amentoflavone, anticancer, docking, robustaflavone, scaffold



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EVALUATING THE SAFETY OF HERBAL MEDICINES: CURRENT CHALLENGES AND REGULATORY PERSPECTIVES

Rausan Zamir ^a, ²Nazmul Islam ^b, ¹Mamun-Ar Rashid ^a, Shahed Zaman ^a

^a Department of Chemistry, University of Rajshahi, Rajshahi- 6205, Bangladesh

^b Department of Textile Engineering, Faculty of Engineering, Daffodil International University, Dhaka, Bangladesh

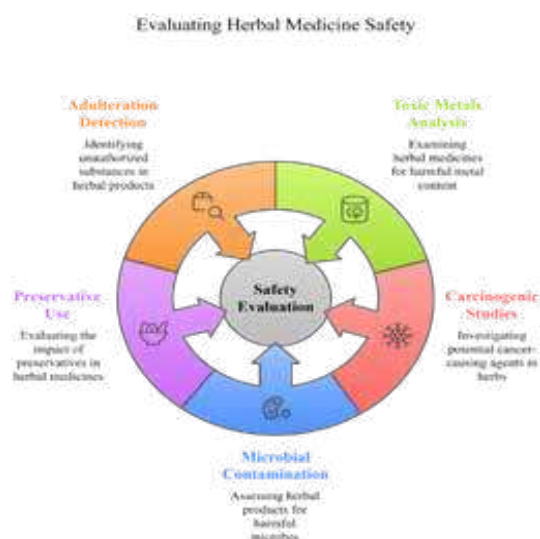
*Corresponding author: rsnzamir@gmail.com

Abstract

The consumption of herbal medicinal goods and supplements has surged significantly over the past three decades, with around 80% of the global population using them for various aspects of primary healthcare.

With a projected population of 218 million by 2030, Bangladesh is the eighth most densely inhabited nation in the world. The World Health Organisation (WHO) reports that government spending on health is 34%, increasing the likelihood of inequality and that only 3% of GDP is allocated to health services, the lowest amount among 45 Least Developed Countries (LDCs). Due to this gap, a large number of herbal medications are being used for medical purposes despite concerns about their safety, potential negative health effects, and a lack of scientific data. Contaminants in herbal drugs are being reported in different scientific literature elsewhere with scarce investigation from locally formulated herbal drugs. However, adverse health risks due to the consumption of herbal drugs are reported in different national electronic and print media on a regular basis. A safety assessment is being conducted with funding from the International Science Program (ISP) to consider these findings and produce scientific data on herbal medications formulated in Bangladesh. Investigations into toxic metals, carcinogenic and non-carcinogenic analysis, microbiological contamination evaluation, preservative investigation, and potential adulteration in various herbal remedies used in Bangladesh were conducted to achieve the objectives. Positive findings from the investigations encourage the appropriate organization to monitor the formulations closely.

Keywords: Herbal medicines, safety assessment, adverse health effects, toxic metals, microbial contamination, adulteration



HARNESSING SUSTAINABLE RESOURCES FOR RESEARCH AND INNOVATION

Zainab Ngaini, Mohamad Azmeer Hissam, Siti Nur Aqilah Makshut, Mohamad Asri Jefferi

Faculty of Resource Science and Technology, University Malaysia Sarawak, 94300 Kota Samarahan, Sarawak

Email: nzainab@unimas.my

Abstract

In the pursuit of a sustainable future, green chemistry plays a pivotal role in harnessing nature's potential to address environmental challenges and depleting non-renewable resources. This talk explores innovative methodologies in sustainable chemistry, focusing on drug discovery and green chemistry to drive environmental conservation and societal well-being. This talk will highlight groundbreaking studies on utilizing natural resources, showcasing the successful applications of organic chemistry/synthesis in industries such as solar cells, liquid crystals, energy storage, and pharmaceuticals. It will emphasize green chemistry principles, including the use of renewable feedstocks and the reduction of waste. We will also address the challenges and opportunities in scaling up these innovations, emphasizing the need for further research and investment in sustainable development. By leveraging nature's potential through sustainable chemistry, we can inspire a new generation of scientists and policymakers to commit to a greener and more resilient future.

EXPLORING THE ROLE OF SAFFRON IN REVERSE CHOLESTEROL TRANSPORT: A NOVEL APPROACH TO ATHEROSCLEROSIS INTERVENTION

Yasmin Mohd Zainal Abidin Shukri¹, Che Puteh Osman², Siti Azma Jusoh³,
Noor Alicezah Mohd Kasim^{1,4*}

¹Cardiovascular Advancement and Research Excellence Institute (CARE Institute), Universiti Teknologi MARA

²Atta-ur-Rahman Institute for Natural Product Discovery (AuRIns), Universiti Teknologi MARA

³Department of Life Sciences, Faculty of Pharmacy, Universiti Teknologi MARA

⁴Department of Pathology, Faculty of Medicine, Universiti Teknologi MARA

*Corresponding author: noor202@uitm.edu.my

Abstract

Natural products have long been explored for their therapeutic potential in disease management. Saffron (*Crocus sativus* L.), a medicinal plant rich in bioactive compounds, has gained attention for its cardioprotective effects, particularly in modulating lipid metabolism and reverse cholesterol transport (RCT). This study evaluates saffron's effects on cholesterol-regulating genes via quantitative real-time Polymerase Chain Reaction (qRT-PCR) and investigates the molecular interactions of its bioactive compounds through molecular docking studies. Thirty-five New Zealand White rabbits were fed a 1% high-cholesterol diet for 8 weeks to induce atherosclerosis, followed by treatment in five groups: baseline, statins, placebo, and saffron extract (SE) at 50 mg/kg/day (S50) and 100 mg/kg/day (S100) for another 8 weeks. Liver tissues were analyzed for ABCA1, SR-B1, and PPAR- γ gene expression via qRT-PCR (2- $\Delta\Delta C_t$ method). Molecular docking was performed using MolModa (AutoDock Vina) with compound structures retrieved from PubChem, and receptor-ligand interactions were visualized using PyMOL and PoseEdit. Our findings demonstrated that S100 dose significantly upregulated SR-B1 expression (8.34-fold, $p < 0.05$), surpassing statins (5.52-fold), suggesting enhanced cholesterol clearance. ABCA1 expression was highest in S50 (4.36-fold), indicating its role in cholesterol efflux. PPAR- γ expression was also elevated in saffron-treated groups, supporting its involvement in lipid metabolism regulation. Molecular docking revealed that crocetin (-7.75 kcal/mol) had the strongest affinity for PPAR- γ , while dimethylcrocetin (-8.72 kcal/mol) exhibited the highest binding to SR-B1, demonstrating its role in cholesterol efflux and clearance, which is crucial in enhancing RCT. Quercetin (-8.35 kcal/mol) was the top binder to ABCA1, reinforcing its role in cholesterol efflux. In conclusion, our findings highlight saffron's potential in enhancing reverse cholesterol transport (RCT) and reducing atherosclerosis progression by modulating key lipid metabolism pathways. While promising, further research is needed to refine its therapeutic potential through clinical trials and mechanistic studies. Future directions may focus on optimizing saffron's efficacy in atherosclerosis prevention and treatment.

Keywords: Saffron, atherosclerosis, RCT, gene expressions, molecular docking.



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PHENOXYMETHYLKETONE WARHEADS CREATE POTENT DUAL-MODE PEPTIDOMIMETIC INHIBITORS AGAINST SARS-COV-2

Miriam R.B. Porzberg^a, Willem H.C. Titulaer^a, Lorenzo Cavina^a, Martin C. Feiters^a, Daniel Gironés^{a,b}, Floris P.J.T. Rutjes^{a,*}

^a Institute for Molecules and Materials, Radboud University
Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

^b Protinhi Therapeutics, Transistorweg 5, 6534 AT Nijmegen, The Netherlands.

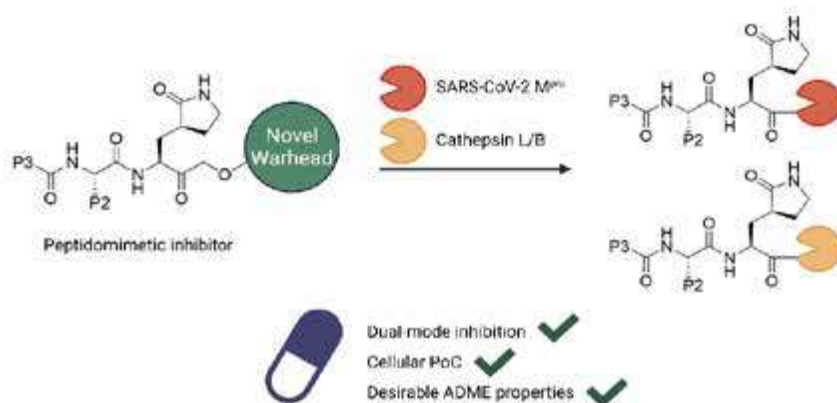
*Corresponding author: floris.rutjes@ru.nl

Abstract

To battle SARS-CoV-2 and future coronavirus outbreaks, peptidomimetic protease inhibitors against the SARS-CoV-2 main protease (Mpro) as well as host proteases cathepsin L and cathepsin B form an efficient and attractive strategy in antiviral drug discovery. Dual mode antiviral small molecules inhibiting both viral entry and viral replication simultaneously have gained more attention recently and could be suitable alternatives to the highly specific Mpro and cathepsin (CTS) inhibitors currently on the market and in clinical trials.

Herein, we examine the design and synthesis, inhibitory activity, in vitro ADME properties, metabolic stability and pharmacokinetics of a library of peptidomimetic inhibitors bearing a potent phenoxyethyl ketone warhead. Our compounds are nanomolar inhibitors of both Mpro and CTSL/CTSB, and efficiently inhibit SARS-CoV-2 in cellular reporter and functional assays.¹ As CYP-dependent metabolism is one of the major challenges in further drug development of potent protease inhibitors, we evaluated the inhibitory activity of the metabolite, as well as the impact of co-administration with ritonavir. Furthermore, results from the most promising compound evaluated in a hamster SARS-CoV-2 infection model will be discussed. Taken together, we report a promising lead compound against SARS-CoV-2 with attractive properties to be further pursued in preclinical studies.

Keywords: Covid, Antiviral small molecules, Dual inhibition, Peptidomimetics, Covalent inhibition



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ENRICHING FLAVONOIDS: SUSTAINABLE VALORIZATION OF KENAF (*HIBISCUS CANNABINUS* L.) BYPRODUCTS FOR THE DEVELOPMENT OF NATURAL THERAPEUTIC AGENTS IN WOUND HEALING

Raghad Yousef Ali Al-Jawarneh^{a,b*}, Fauziahanim Zakaria^c, Mohamad Shazeli Che Zain^{a,b*}

^aBioresource Technology Division, School of Industrial Technology, Universiti Sains Malaysia, Gelugor, Malaysia.

^bPhytochemistry and Phytotechnology Research Group (PhytoRG), Universiti Sains Malaysia, Gelugor, Malaysia

^cDiscipline of Pharmaceutical Chemistry, School of Pharmaceutical Sciences, Universiti Sains Malaysia, Gelugor, Malaysia.

*Corresponding author: shazeli@usm.my

Abstract

Diabetes mellitus affects millions worldwide, with approximately 340 million diagnosed cases. A major complication is impaired wound healing, impacting nearly 25% of diabetic patients. Conventional treatments, such as medications, dressings, and surgeries, are costly and may cause side effects. Thus, natural alternatives like flavonoids are gaining interest for their antioxidant, anti-inflammatory, and antimicrobial properties. Kenaf (*Hibiscus cannabinus*), a flavonoid-rich plant, shows promise for diabetic wound healing. This study aimed to extract and enrich flavonoids from kenaf and evaluate their antioxidant and wound healing properties using zebrafish models. Flavonoid purification was performed using macroporous adsorbent resin chromatography, optimizing pH, contact time, concentration, temperature, and desorption solvents. Optimal adsorption occurred at pH 7, equilibrium was reached in 1440 minutes, and adsorption increased with temperature, following a pseudo-second-order kinetic model and the Freundlich isotherm. Desorption using 95% ethanol (HP-20), 60% ethanol (XAD-4), and 20% ethanol (LXA-817) enriched flavonoid concentrations by 11-fold, 10-fold, and 5-fold, respectively. HPLC-MS/MS analysis identified key flavonoids, including kaempferol derivatives, apigenin, quercetin, and myricetin. Antioxidant assays (DPPH, ABTS, FRAP) confirmed strong radical scavenging activity. To assess wound healing efficacy, zebrafish were treated with kenaf flavonoid-enriched extract (KFEE). Toxicity tests showed an LC_{50} of 71 mg/mL, with no mortality below 50 mg/mL. Diabetic zebrafish were induced with 2% glucose for four weeks before wound creation. Treatment groups included control, positive control (allantoin), and KFEE (6.25 mg/L and 25 mg/L). By day 30, normal zebrafish treated with high- and low-dose KFEE achieved 95% and 90% wound closure, outperforming the positive control (85%). In diabetic zebrafish, high- and low-dose KFEE achieved 80% and 75% closure, exceeding positive (67%) and negative (60%) controls. KFEE significantly improved diabetic wound healing, demonstrating its potential as a natural therapeutic.

Keywords: kenaf; enrichment; flavonoid; diabetic wound; zebrafish

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TOCOTRIENOL ISOMERS AS POTENTIAL ANTI-ATHEROGENIC AGENTS: A MOLECULAR DOCKING STUDY TARGETING E-SELECTIN, ICAM-1, AND VCAM-1

Hazirah Watikah Abdah¹, Siti Azma Jusoh², Noorul Izzati Hanafi¹, Suhaila Abdul Muid^{1,3}, Noor Alicezah Mohd Kasim^{1,4}

¹Cardiovascular Advancement and Research Excellence Institute (CARE Institute), Universiti Teknologi MARA

²Department of Life Sciences, Faculty of Pharmacy, Universiti Teknologi MARA

³Department of Biochemistry & Molecular Medicine, Faculty of Medicine, Universiti Teknologi MARA

⁴Department of Pathology, Faculty of Medicine, Universiti Teknologi MARA

*Corresponding author: noor202@uitm.edu.my

Abstract

Atherosclerosis is a chronic inflammatory disease characterized by endothelial dysfunction and leukocyte adhesion, mediated by cell adhesion molecules such as E-selectin, intercellular adhesion molecule-1 (ICAM-1), and vascular cell adhesion molecule-1 (VCAM-1). Tocotrienols, a subgroup of vitamin E, exhibit potent antioxidant and anti-inflammatory properties, suggesting their potential role in mitigating atherosclerosis. This study aims to evaluate the binding of tocotrienol isomers (α -, β -, γ -, and δ) to three adhesion proteins: E-selectin, ICAM-1, and VCAM-1. The study employed the molecular docking method to predict the binding of tocotrienols to the target proteins. The three-dimensional (3D) structures of E-selectin, ICAM-1, and VCAM-1 were retrieved from the *UniProt* database, while tocotrienol isomers were obtained from *PubChem*. The binding pockets of the target proteins were selected based on the druggability scores computed by the *DogSiteScorer* program. Subsequently, the docking experiment was conducted using *MolModa*, an automated molecular docking platform based on *Autodock Vina*. The results for each compound were selected based on the top binding affinity to the potential binding pockets. Inter-molecular analysis between tocotrienols and binding pocket residues was performed using *Discovery Studio*, and visualized using *Pymol*. Molecular docking analysis demonstrated that all tocotrienol isomers bind to the predicted binding pockets of the key adhesion proteins. Overall, all tocotrienol isomers exhibited strongest binding affinities to VCAM-1 with average affinity of -7.3 kcal/mol. Meanwhile for E-selectin and ICAM-1, the binding affinities of tocotrienol isomers are between -6.8 to -5.3 kcal/mol. Among all the isomers, α -tocotrienol displayed the highest binding affinity to all target proteins: VCAM-1 (-7.5 kcal/mol), ICAM-1 (-6.8 kcal/mol) and E-selectin (-6.7 kcal/mol). The findings highlight the potential role of tocotrienol in modulating cell adhesion processes, which may have implications for therapeutic interventions targeting inflammatory and vascular-related pathways. Further experimental validation is warranted to confirm these *in silico* predictions and explore their biological significance.

Keywords: Tocotrienol, atherosclerosis, molecular docking, endothelial adhesion biomarker

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BIOLOGICAL EFFICACY OF TETRAHYDROCURCUMIN ANALOGS: IMPLICATIONS FOR ANTIAGING SKINCARE

Ritmaleni^{a,b,*}

^aCurcumin Research Center, Faculty of Pharmacy, Gadjah Mada University, Yogyakarta, Indonesia.

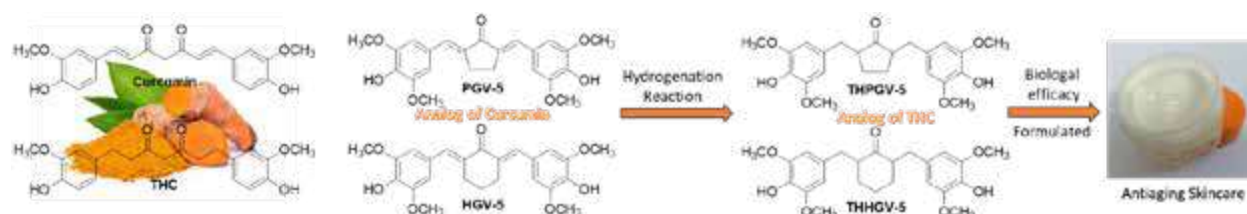
^bLaboratory of Medicinal Chemistry, Faculty of Pharmacy, Gadjah Mada University, Yogyakarta, Indonesia.

*Corresponding author: ritmaleni@ugm.ac.id

Abstract

One important curcumin derivative, tetrahydrocurcumin (THC), is well known for its strong biological characteristics, such as its anti-inflammatory and anti-oxidant activities, which make it a viable option for cosmetic use. This study examines various novel THC analogs' biological effectiveness and their uses in anti-aging skincare products. Tetrahydropentagamavunon (THPGV-5) and Tetrahydrohexagamavunon (THHGV-5) are two of them. These two substances are generated from Hexagamavunon-5 (HGV-5) and Pentagamavunon-5 (PGV-5), which are curcumin analogs. Beginning with the reaction condensation between the appropriate aldehyde of PGV-5 and HGV-5 with cyclopentanone or cyclohexanone at room temperature, the synthetic method for their synthesis was initiated. Next, H₂ gas and Pd/C act as catalysts to hydrogenate PGV-5 and HGV-5 for two hours at room temperature.¹ The color of the reaction mixture changes from yellow to transparent in this hydrogenation process, making it an auto-indicator reaction. For a number of applied curcumin analogs, moderate to high yields were obtained. Then evaluation of their biological activities including antioxidant and antibacterial properties.² When compared to vitamin E, THPGV-5 and THHGV-5 have superior antioxidant activity. As a result, THPGV-5 or THHGV-5 was used as the active ingredient in these two compounds' antiaging formulation. The concentrations of 0,010% w/w, 0,015% w/w, and 0,020% w/w were used in the formulation of the items. The physical characteristics and properties of the studied formulae, such as organoleptic, pH, adhesion, dispersion, and cream viscosity, supported this inference. Additionally, the formulae' in vitro and in vitro testing were conducted. Based on the thickness of the collagen in rat skin, the antiaging effect increases with the concentration of the active ingredient. The rabbit skin did not get irritated by any of the antiaging product compositions. To conclude, formulations including THPGV-5 or THHGV-5 as the active ingredient show promise for future development as antiaging ingredients in skincare products.³⁻⁵

Keywords: Antiaging skincare, Biological efficacy, Tetrahydrocurcumin analog, THPGV-5, THHGV-5



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ANTICANCER ACTIVITY AND CELL DEATH MECHANISM OF HETEROLEPTIC BIMETALLIC RUTHENIUM(II,III) COMPLEXES AGAINST HUMAN BREAST CANCER SUB-TYPES

Siyabonga Ngubane^{a,*}, Sharon Prince^b, Nirvashi Autar^a, Thato Medupe^a

^a University of Cape Town, Department of Chemistry, Rondebosch, 7701, Cape Town, South Africa,

^b University of Cape Town, Department of Human Biology, Observatory, 7935, Cape Town, South Africa

*Corresponding author: siyabonga.ngubane@uct.ac.za

Abstract

Diruthenium complexes have emerged as propitious anticancer metallodrugs, owing to their stable topologies, redox-active metal centers and hence, the ability to interact with redox biological molecules. [1] These molecules include reactive oxygen species (ROS), by-products of cellular metabolism, known to instigate oxidative stress in the cells. The cellular homeostatic control of ROS is regulated by the antioxidant glutathione (GSH). The disruption of the interactions between these two biological small molecules is reported to trigger various types of apoptotic cell death pathways due to an imbalance in the cellular redox environment.[2] Novel mixed-ligand diruthenium complexes of the type $[\text{Ru}_2(\text{O}_2\text{CCH}_3)_3(\text{Rap})(\text{DsIm})_n]\text{Cl}$ where R = 2-F, 4-F, 4- CH_3 substituents on an anilinopyridinate (ap) ligand and n = 1 (**C1a** – **C3a**) or 2 (**C1b**) decorated axially with a biologically-active dansyl-imidazole (DsIm) ligand have demonstrated promising anti-cancer activity and affinity ruthenium complexes.[3] The afore-mentioned Ru_2^{5+} complexes also have affinity for GSH ($K = 10^7 - 10^{10} \text{ M}^{-1}$), oxidizing it to the inactive, GSSG upon binding *via* a Ru metal-reduction reaction. A cell-free dichlorofluorescein (DCF) assay indicate that the complexes are oxidised by hydrogen peroxide to generate hydroxyl radicals as the ROS. These proposed metallodrugs also presented *in vitro* cytotoxic properties as well as selectivity towards different breast cancer cells with **C1b** found as the most potent ($\text{IC}_{50} = 27 \mu\text{M}$ in MCF-7; $43 \mu\text{M}$ in MDA-MB-231u) in cytotoxicity and has good selectivity over the non-malignant, MCF-12A cells. Furthermore, **C1b** also influenced the *in vitro* GSH and ROS level in breast cancer cells, consistent with redox-mediated interactions observed under cell-free conditions.

Keywords: redox-induced cancer cell death, diruthenium complexes, chemotherapy, glutathione, ROS

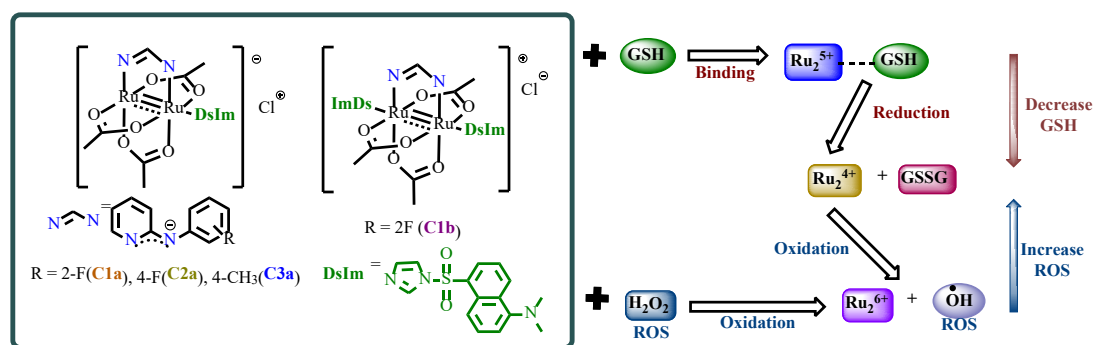


Figure 1. The dansyl-based diruthenium complexes and their interactions with redox molecules.

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MALIC ENZYME INHIBITION OF PYRIMIDINE DERIVATIVES FOR PANCREATIC CANCER TREATMENT

Shubham Mehta¹, Gautam Patel^{1*}

¹*Chemistry Department, Parul Institute of Applied Science, Parul University, Vadodara-391760, Gujarat, India.*

**Corresponding author: shubham.research18@gmail.com*

Abstract

Pancreatic cancer, predominantly pancreatic ductal adenocarcinoma (PDAC), is the most rapidly progressing, uncontrolled, and fatal malignancy worldwide. Current research indicates that malic enzymes, especially ME2 and ME3, play a vital role as metabolic regulators in the proliferation of pancreatic cancer. A malic enzyme facilitates the conversion of malate to pyruvate, the production of NADPH, and lipid biosynthesis, all of which are crucial for cancer growth. Ongoing research has identified ME2 with the deletion of the tumor suppressor gene SMAD and its family member 4 (SMAD4), which is associated with 40% of PDAC patients. Additionally, in SMAD4/ME2/PDAC cells, the function of the ME2 enzyme is substituted by ME3, which placed in the mitochondria, thus necessitating the targeted inhibition of ME3 cell growth. Hence, the present study describes improvements in pyrimidine derivatives to enhance them in vitro cytotoxicity, inhibitory effect, and metabolic stability in pancreatic cancer. Herein, we report the synthesis and characterization of novel 1,3-diazine via Buchwald-Hartwig cross-coupling of aryl halides and secondary amines, followed by a structure-activity relationship (SAR) study. Furthermore, molecular docking studies have been performed on the synthesized 1,3-diazine derivatives of the reported Olaparib drug with PDB IDs (1GZ3, 1QR6, 8EYN, 1PJ3) to check binding interactions. Moreover, we checked the inhibition assay on PDAC cell lines such as BxPC-3, PANC-1, CFPAC-1, and MIA PaCa-2 with the 1,3-diazine derivatives.

Keywords: Buchwald-Hartwig cross-coupling, Pancreatic Cancer, Malic enzyme inhibition, Molecular docking study, SAR activity.

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PYRIDINE DERIVATIVES TARGETING ACETYLCHOLINESTERASE INHIBITION IN ALZHEIMER'S DISEASE

Iti Patel¹, Gautam Patel^{1*}

^{1*}Chemistry Department, Parul Institute of Applied Science, Parul University, Vadodara-391760, Gujarat, India.

*Corresponding author: itipatel1109@gmail.com

Abstract

Alzheimer's disease is the most common neurological disorder worldwide. The most progressive cause of Alzheimer's disease is the accumulation of amyloid plaques and increased tau tangle protein in the brain, which causes gradual death of the neuron cells. In recent years, there have been 6.9 million elderly people suffering from Alzheimer's disease. According to the pathology of AD, the reactive oxygen species (ROS) that are made by the amyloid beta peptide cause plaques to form. The cholinergic neurons then increased the activity of acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), which led to cognitive decline. Because of that need to plan a strategy to inhibit AChE and BChE, followed by the heterocyclic organic synthetic pathway. Apart from that, the pyridine heterocyclic derivative is strongly effective on the inhibition of AChE and BChE to stop AD. The present study introduced the recent advances in the synthesis of pyridine derivatives via cross-coupling reactions, functional group modification, and the Schiff base pathway to enhance the cholinesterase inhibition effect. Moreover, the structural activity relationship (SAR) of synthesized pyridine derivatives is investigated to show their selectivity, potency, and pharmacological activity to treat AD. Additionally, we performed the in vitro biological evaluation of synthesized pyridine derivatives on the AChE cell line, such as SH-SY5Y and IMR-32, to check inhibition of AChE.

Keywords: SAR of pyridine derivatives, Schiff base synthesis, Alzheimer's disease (AD), AChE inhibition.

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COMPREHENSIVE METABOLITE PROFILING, CYTOTOXICITY EVALUATION, AND ANTINOCICEPTIVE ACTIVITY OF OPTIMIZED KRATOM LEAVES EXTRACT USING ACCELERATED SOLVENT EXTRACTION TECHNIQUE

Thiruvethan Karunakaran^{a*}, Nurul Najwa Rusmadi^a, Faiqah Ramli^b, Intan Safinar Ismail^c, Rameshkumar Santhanam^d, Mohamad Hafizi Abu Bakar^e, Azira Muhamad^f, and Surash Ramanathan^a

^aCentre for Drug Research, Universiti Sains Malaysia, 11800 USM, Pulau Pinang, Malaysia

^bDepartment of Bioprocess & Polymer Engineering, School of Chemical & Energy Engineering, Faculty of Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Malaysia,

^cLaboratory of Natural Products, Institute of Bioscience, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia,

^dBioSES Research Interest Group, Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, Kuala Nerus 21030, Terengganu, Malaysia,

^eBioprocess Technology Division, School of Industrial Technology, Universiti Sains Malaysia, Gelugor 11800 USM, Penang, Malaysia,

^fMalaysia Genome and Vaccine Institute, National Institutes of Biotechnology Malaysia, 43000 Kajang Selangor

*Corresponding author: thiruvethan@usm.my

Abstract

Kratom (*Mitragyna speciosa*), locally known as ketum, has gained attention for its potential therapeutic benefits in pain management and addiction treatment^{1,2}. The bioactive properties of kratom are influenced by the extraction techniques used to enhance and enrich the content of key compounds³. This study aimed to optimize the extraction conditions for mitragynine, phenolic acids, and flavonoids content from kratom leaves using the Accelerated Solvent Extraction (ASE) method, which is known for its efficiency in improving metabolite yield³. Fresh kratom leaves were harvested from an informal plantation in Bukit Mertajam, Penang, and freeze-dried. ASE optimization was performed using a two-step approach, first, the One-Factor-At-A-Time (OFAT) method was used to assess individual extraction parameters, followed by Box-Behnken Design (BBD) and Response Surface Methodology (RSM) for further optimization. The optimal conditions were determined to be 8 minutes of extraction at 60°C with 40% ethanol, yielding 4.66% mitragynine, 212.69 GAE mg/g total phenolic content, and 126.13 QE mg/g total flavonoid content. The optimized kratom leaves extract was then subjected to cytotoxicity evaluation (MTT assay), antinociceptive assessment (hot plate test), and detailed metabolite profiling using ¹H-NMR, 2D J-resolved NMR, and UPLC-ESI-QTOF-MS/MS. Cytotoxicity results indicated selective activity against HepG2 liver cancer cells with minimal toxicity towards normal liver cells (HL-7702) at concentrations ranging from 3.125 µg/mL to 200 µg/mL. Antinociceptive evaluation in Swiss albino mice demonstrated significant analgesic effects at doses of 100, 200, and 500 mg/kg. Metabolite profiling identified key phytochemicals, including indole alkaloids (mitragynine, speciogynine, paynantheine), phenolic acids, and flavonoids such as quercetin and rutin. These findings demonstrate the potential of optimized ASE extraction to yield kratom extracts with significant pharmacological properties and suggest further research is needed to refine extraction methods and explore kratom's therapeutic applications.

Keywords: Kratom; Mitragynine; Accelerated Solvent Extraction (ASE); Extraction optimization

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SPONTANEOUS FORMATION OF 17 AMINO ACIDS USING WATER RADICAL CATIONS MEDIATED NITROGEN AND CARBON DIOXIDE

Rui Su^{a,b}, Xiaoping Zhang^{a,c}, Shuxiang Yan^a, Xuwen Chen^a, Wenbo Zhang^d, Ruonan Zhao^a, Tenggao Zhu^a, Yutong Han^b, Xinyu Li^b, Jiaquan Xu^c, Dapeng Liang^b, Huanwen Chen^{a,*}

^a Jiangxi University of Chinese Medicine

^b Jilin University

^c East China University of Technology

^d Changchun University of Chinese Medicine

*Corresponding author: chw8868@gmail.com

Abstract

The origin of life remains one of science's most enduring mysteries. Amino acids, as fundamental components of proteins, are key to understanding the chemical evolution that led to life on Earth¹. Previous studies have focused on the synthesis of amino acids using reducing gas mixtures, but recent consensus suggests that the early Earth atmosphere was primarily composed of CO₂, N₂, and H₂O². In this study, we investigated the abiotic synthesis of amino acids from a mixture of nitrogen, carbon dioxide, and water vapor under atmospheric pressure and room temperature conditions, without the use of chemical catalysts. A custom-designed experimental setup was used to generate water radical cations by electrical discharge³, which then reacted with N₂ and CO₂ in a reaction chamber. Using multi-stage tandem mass spectrometry (MS), liquid chromatography-mass spectrometry (LC-MS), and isotope labeling techniques, we identified and quantified 17 amino acids, including glycine, alanine, and valine. Among these, glycine was produced at the highest rate (22.7 µg/cm²/h), approximately 100 times more than other amino acids. Notably, the yields were significantly affected by the order of interactions between the water radical cations and nitrogen before carbon dioxide. The synthesis process was verified by fragmentation patterns matching standard amino acids and high-resolution mass spectrometry data, confirming the amino acids formed were identical to commercially available standards. Our findings demonstrate that amino acids can be synthesized abiotically from simple atmospheric gases under conditions analogous to early Earth, providing new insights into potential pathways for the origin of life and suggesting further applications for advanced scientific research.

Keywords: origin of life, amino acids, abiotic synthesis, water radical cations, mass spectrometry

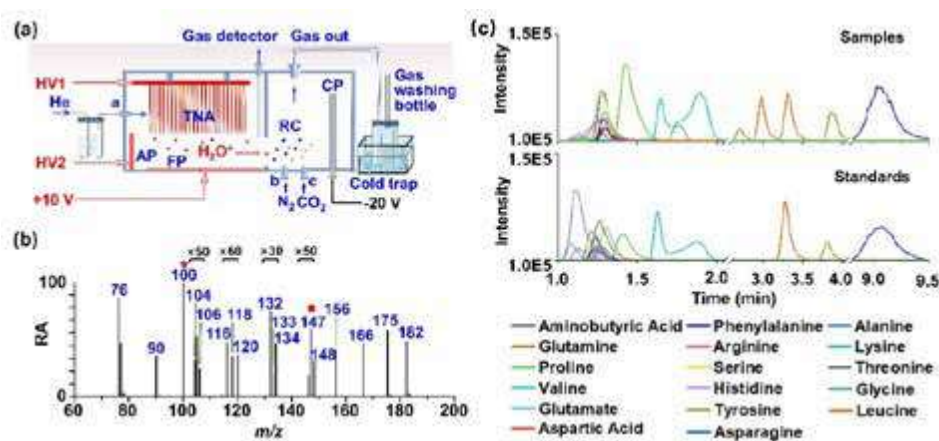


Fig. Ambient formation of amino acids using water, nitrogen and carbon dioxide.

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MIXONAT – DRIVEN NATURAL PRODUCT RESEARCH: UNLOCKING BIOACTIVE TREASURES

Mohamad Nurul Azmi^{a,*}, Séverine Derbré^b, Marc Litaudon^c, Khalijah Awang^d

^a*Natural Products and Synthesis Organic Laboratory (NPSO), School of Chemical Sciences, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia.*

^b*Universite Angers, SONAS, SFR QUASAV, Angers F-49000, France*

^c*Institut de Chimie des Substances Naturelles, CNRS-ICSN UPR 01, Université Paris-Sud 11, Av. de la Terrasse, 91198 Gif-sur-Yvette, France*

^d*Department of Chemistry, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia*

*Corresponding author: mnazmi@usm.my

Abstract

Natural products have long been a rich source of bioactive compounds, yet their exploration is often hindered by the time-consuming process of isolation and redundant rediscovery of known metabolites. To overcome this challenge, we introduce MixONat, a strategic approach that integrates ¹³C NMR-based dereplication with targeted isolation to accelerate natural product discovery. By streamlining structure elucidation at an early stage, MixONat significantly enhances the efficiency of identifying novel bioactive compounds.

In this presentation, we showcase the application of MixONat through two case studies. The first focuses on five species of *Diospyros*, a genus known for its chemical diversity. Leveraging MixONat, we rapidly identified secondary metabolites and evaluated their potential as anti-dengue agents. Through molecular docking studies, we explored their interactions with key viral proteins, uncovering promising candidates for further pharmaceutical development. The second case study shifts to the genus *Aglaia*, a rich source of triterpenoids with potential cytotoxic properties. Using MixONat, we efficiently dereplicated known metabolites and selectively targeted novel triterpenes for isolation. Bioactivity screening against cancer cell lines revealed potent cytotoxic effects, emphasizing the therapeutic potential of these compounds.

These findings underscore the application of MixONat as a transformative strategy in natural product research, enabling rapid dereplication, targeted isolation, and bioactivity-driven discovery. By reducing the time and resources required for metabolite characterization, this strategy paves the way for more efficient drug discovery from nature's vast chemical reservoir.

Keywords: MixONat; ¹³C-NMR dereplication; Rapid identification; *Diospyros*; *Aglaia*

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AUGMENTED DOCKING PIPELINES: LEVERAGING MACHINE LEARNING IN TEMPLATE-BASED NNRTI SCREENING MODELS

Swagata Gupta^{*a}

^aDepartment of Chemistry, Govt. Holkar (Model, Autonomous) Science College, Indore, M.P., India

^{*}Corresponding Author Email id: swagatagupta28@gmail.com

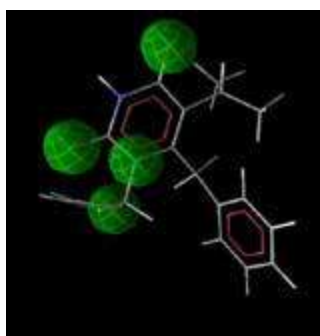
Abstract

HIV drug resistance presents a persistent challenge in antiviral therapy, especially concerning non-nucleoside reverse transcriptase inhibitors (NNRTIs), which are crucial to current treatment regimens. This study introduces a machine learning-integrated, template-based molecular docking strategy to identify potent NNRTIs by analyzing the binding behavior of HEPT analogues within the non-nucleoside inhibitor binding pocket (NNIBP) of HIV-1 reverse transcriptase (RT). Utilizing the crystal structure of HIV-1 RT bound to MKC-442 (PDB ID: 1RT1), pharmacophore templates were derived to guide docking simulations based on steric, hydrophobic, and hydrogen bonding features. Docking scores and binding affinities were correlated with biological activity (pIC₅₀) using linear regression and cross-validation models, achieving strong predictive performance ($r^2 > 0.88$, MSE < 0.2). Structural analysis highlighted consistent hydrogen bonding at the pyrimidine 3-N site (with LYS101) and significant π - π stacking with PHE227 and PRO236. Electrostatic interactions also contributed to binding stabilization in specific analogues. Furthermore, AI-guided datamining of the PubChem database retrieved novel hit compounds with superior predicted binding affinities. This integrated computational workflow improves docking accuracy and predictive modeling, offering a valuable tool for the rational design of next-generation NNRTIs with improved resistance profiles and broader applicability in antiviral drug discovery.

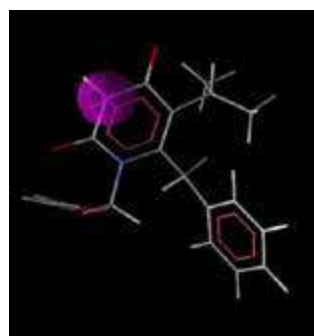
Keywords: Template-based docking, Machine learning, HEPT analogues, NNRTIs, Virtual screening

Figure 1-a-d: Templates showing different groups for MKC-442.

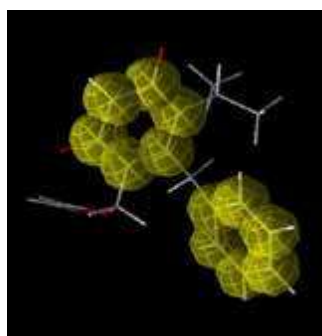
1-a Hydrogen Acceptor (HA)



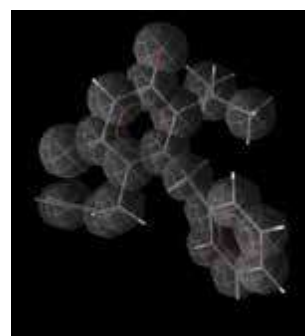
1-b Hydrogen Donor (HD)



1-c Ring (R)



1-d Steric (S)



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DEEP COMPLEX PROCESSING OF SIBERIAN PLANT WASTE AS A WAY TO ACHIEVE THE SUSTAINABLE DEVELOPMENT GOALS

Elena Avdeenko^{a,*}, Pavel Zaikin^a

^a N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry of the Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia

*Corresponding author: avdeenko@nioch.nsc.ru

Abstract

Siberian plants, in particular fir, cranberry, chokeberry and birch, contain a large number of different valuable organic compounds. A large amount of waste remains containing a large amount of biologically active substances after processing of these trees or berries. Deep complex processing of waste plant materials will increase the environmental friendliness of the process, improve economic efficiency and obtain a large list of critical components that can help achieve sustainable development goals:

- **SDG 2 «Zero hunger».** Fir triterpenoids allow to achieve higher plant yields and increase their resistance to diseases¹. The plant matrix of Siberian fir or berries can be used as a melioration material, a substrate for growing in agriculture or as a vitamin supplement for cattle².
- **SDG 3 « Good health and well-being».** Siberian fir and berries contain vitamin complexes and biologically active compounds that have a significant beneficial effect on human health^{3,4}. It can be a component of functional food and a source of natural dyes and antioxidants. Triterpenoid derivatives from berries (ursolic acid) and birch bark (betulin) demonstrate high health-promoting, antiviral and antitumor activity^{3,5,6}.
- **SDG 12 «Responsible consumption and production».** Recycling of logging and food industry waste allows for more efficient use of natural resources. And while plant-based raw materials are a renewable resource, responsible production is critical to the modern world. Rational deep complex processing of plant waste will not only reduce resource consumption, but also produce a greater quantity of critically important and useful products from previously disposed waste.

Thus, the introduction of an integrated approach to processing Siberian plant waste will allow obtaining a large number of valuable organic substances and will have a noticeable impact on many areas of human life. As a result, using the unique properties of Siberian plants will help bring closer the achievement of some sustainable development goals.

Keywords: Siberian plant waste, waste processing, sustainable development goals, triterpenoids



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HEALTH AND NUTRITIONAL BENEFITS OF THE COCONUT FOR FOOD SECURITY

Dr. Fabian M. Dayrit ^{a,*}, Dr. Jelfina C. Alouw ^b

^aDepartment of Chemistry, Ateneo de Manila University, Quezon City, Philippines

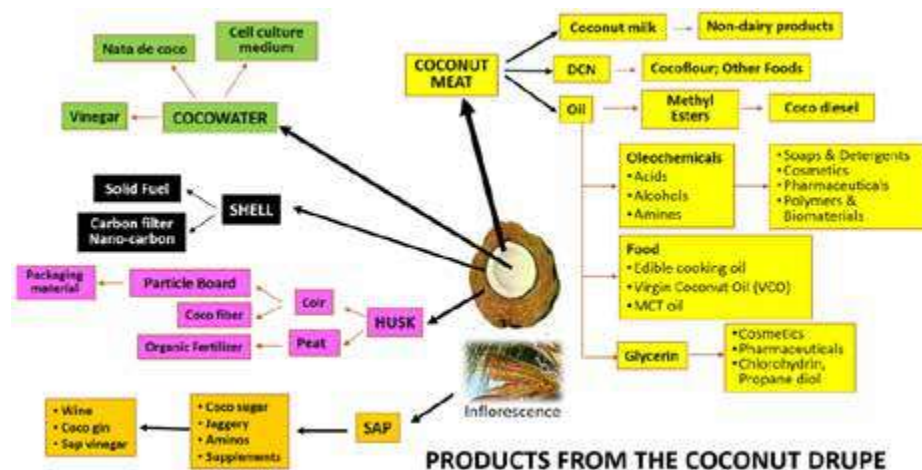
^bInternational Coconut Community, Jakarta, Indonesia

*Corresponding author: fdayrit@ateneo.edu

Abstract

The coconut provides numerous health and nutritional benefits that can contribute significantly to food security especially in the Tropics. This presentation focuses on the coconut meat, coconut oil and coconut water. Coconut meat contains all of the nine essential amino acids. It contains the highest amount of medium-chain fatty acids among all food sources, is low in carbohydrates and sugars, and contains no cholesterol. Two nuts can provide sufficient energy for one person per day if this is all that this person eats. Traditional and historical accounts describe the coconut as nutritious food even in times of famine. The coconut is a heart-healthy antidote to modern ultra-processed food. The coconut is part of the traditional and culinary diet for 1 billion people in the world. Coconut milk and coconut flour can be obtained from coconut meat. These are sustainable and healthy alternatives to dairy milk and corn flour, respectively. Coconut oil is a unique healthy and therapeutic oil. Coconut oil contains about 50% lauric acid, which has been shown to be antibacterial and antiviral. VCO was shown in two clinical trials to be effective against mild COVID-19. Lauric acid supports a healthy gut microbiota which is essential for health, both in animals and humans. Lauric acid can decrease the use of antibiotics which have led to the development of antibiotic-resistant microorganisms. Lauric acid has also promise in the management of Alzheimer's disease. Coconut water is a unique electrolyte-rich fluid with health benefits. Truly, the coconut is a unique resource with numerous health and nutritional benefits that support SDG2 (No hunger) and SDG3 (Good health and well-being), as well as many of the other UN SDGs.

Keywords: coconut oil, lauric acid, coconut water, SDG 2, SDG 3



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***DODONAEA VISCOSA* FLOWERS: A HAWAIIAN SOURCE OF POTENT ANTIBACTERIAL AND ANTIPROLIFERATIVE EFFECTS IN BREAST CANCER CELLS**

Achara Raksat ^a, Daniel Yee ^a, Young Jin Gi ^b, Supakit Wongwiwatthananut ^c, Leng Kar Chang ^d, Kumu Piilani Kaawaloa ^e, Marisa M. Wall ^f, Jangsoon Lee ^{b,*} and Leng Chee Chang ^{a,*}

^aDepartment of Pharmaceutical Sciences, The Daniel K. Inouye College of Pharmacy, University of Hawai'i at Hilo, Hilo, HI 96720, USA

^bPreclinical Core, Cancer Biology Program, University of Hawai'i Cancer Center, Honolulu, HI 96813, USA

^cDepartment of Pharmacy Practice, The Daniel K. Inouye College of Pharmacy, University of Hawai'i at Hilo, Hilo, HI 96720, USA

^dGeorgia Institute of Science and Research Incorporation, Duluth, GA 30096, USA

^eHawaiian Language/Performing Arts, Kamehameha Schools, Hawai'i Campus, Kea'au, HI 96749, USA

^fDaniel K. Inouye U.S. Pacific Basin Agricultural Research Center, Hilo, HI 96720, USA

*Corresponding author: jlee@cc.hawaii.edu (J.L.) and lengchee@hawaii.edu (L.C.C.)

Abstract

The integration of traditional Hawaiian medicine and modern scientific research highlights the significant therapeutic potential of *Dodonaea viscosa*, commonly known as 'A'ali'i. This traditional Hawaiian medicinal plant was investigated for its bioactive compounds, which possess antimicrobial and antiproliferative properties extracted from its flowers. For centuries, Native Hawaiians have utilized the resilience of this plant to treat various ailments, including toothaches, fever, and skin irritations.¹ The study aimed to discover and characterize the bioactive compounds found in the flower extract of *D. viscosa* flowers. Thirteen compounds were isolated from the methanol extract of fresh *D. viscosa* flowers using chromatography techniques. Their structures were characterized using spectroscopy data, comparing the NMR spectroscopic profiles with previously reported data. Among these, compound **12** (Macarangaflavanone B) displayed potent antimicrobial activity against Gram-positive bacteria, including Methicillin-Resistant *Staphylococcus aureus* (MRSA) and Methicillin-Susceptible *S. aureus* (MSSA), with a low minimum inhibitory concentration (MIC) of 2 µg/mL. Furthermore, the isolated compounds showed dose-dependent anti-proliferative effects on breast cancer cell lines. Notably, inflammatory breast cancer (IBC) cell lines, which represent an aggressive subtype, exhibited higher sensitivity to compound **6** (Santin), with IC₅₀ values ranging from 4.22 µM to 7.73 µM, compared to non-IBC cell lines. The significant activity of Santin against IBC may be attributed to its structural features, particularly the hydroxyl group at the C7 position. These findings underscore the dual therapeutic potential of *D. viscosa* compounds, particularly **12** (Macarangaflavanone B) serving as an antibacterial agent and **6** (Santin) acting as a selective antiproliferative agent against aggressive breast cancer.²

Keywords: *Dodonaea viscosa*, flavonoids, antibacterial activity, breast cancer, antiproliferative effect

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FLAVIN DEPENDENT HALOGENASE FROM THE LICHEN *DIRINARIA* SP.

Nurain Shahera Hasan^{a,b}, Jonathan Guyang Ling^b, Mohd. Faizal Abu Bakar^c,
Wan Mohd Khairulikhshan Wan Seman^c, Farah Diba Abu Bakar^b, Abdul Munir Abdul Murad^b,
Rozida Mohd Khalid^{a*}

^aDepartment of Chemical Sciences, Faculty of Science and Technology.

^bDepartment of Biological Sciences and Biotechnology, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43000 UKM Bangi, Selangor, Malaysia

^cMalaysia Genome and Vaccine Institute (MGVI), National Institute of Biotechnology Malaysia
Selangor, Malaysia

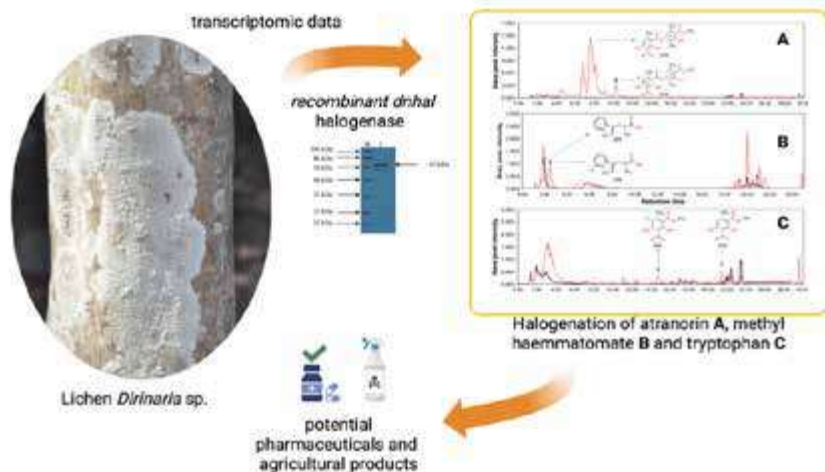
*Corresponding author: rozidakhalid@ukm.edu.my

A

Abstract

Halogenated compounds are widely used for their pharmaceutical and agricultural significance. Recently, there has been an increasing interest in using biocatalyst such as halogenase to modify compounds to enhance chemical diversity. Bioinformatic analysis of the transcriptomic dataset of *Dirinaria* sp. suggested a gene encoding to a non-tryptophan flavin-dependent halogenase (F-Hals), which mainly act on aromatic compounds. The *dnhal* gene was heterologously expressed in *Pichia pastoris* to yield a ~63 kDa purified enzyme that exhibited biocatalytic activity not only towards various aromatic compounds but also toward tryptophan. Tested substrates included methyl haematommate, 3-methyl orsellinic acid, atranorin, benzoic acid, and cinnamic acid. The enzyme showed notable selectivity of chlorination for methyl haematommate and atranorin, consistent with the reports of the isolation of chloroatranorin and methyl chlorohaematommate from *Dirinaria* sp. Further studies need to be done on a variety of aromatic compounds and tryptophan-like substrates to have further understanding of its selectivity. This research marks the beginning of utilizing halogenases as green alternatives as biocatalysts of high-value halogenated compounds.

Keywords: *Dirinaria* sp; halogenase; chlorination; heterologous expression; lichen



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STRUCTURAL CHARACTERIZATION AND BIOACTIVITY EVALUATION OF PLANT-DERIVED POLYSACCHARIDES: A POTENTIAL THERAPEUTIC MANAGEMENT FOR DIABETES

Muhammad Hakimin Shafie*, Muhammad Hasnun Md Yusoff

*Analytical Biochemistry Research Centre (ABrC), Incubator Innovation University (I²U),
sains@usm Campus, Universiti Sains Malaysia, Lebuhr Bukit Jambul, 11900 Bayan Lepas, Penang, Malaysia.*

**Corresponding author: hakiminshafie@usm.my*

Abstract

Polysaccharide extraction using acidic solvents has been extensively studied, demonstrating their effectiveness in achieving high yields. However, overly concentrated acidic solutions can degrade polysaccharide structures, while insufficient acidity often leads to reduced extraction efficiency. To address these limitations, deep eutectic solvents (DES) have emerged as promising alternative extraction media. Their unique ability to form intermolecular and electrostatic interactions offers potential advantages in both extraction efficiency and enhancement of biological activities. In this study, microwave-assisted extraction of polysaccharides from *Micromelum minutum* leaves (MMLP) using DES (MMLP-DES) was compared with conventional citric acid monohydrate (MMLP-CAM). The DES method demonstrated superior performance, requiring 19.83% less microwave power and a 0.78-minute reduction in extraction time, while yielding a 101.20% increase in polysaccharide recovery. Characterization revealed that variations in extraction medium acidity significantly influenced the physicochemical properties of the polysaccharides, including molecular weight, morphology, viscosity, degree of esterification, and monosaccharide composition, all of which impact bioactivity. Functional assays showed that MMLP-DES exhibited markedly higher antioxidant activity (DPPH scavenging: 74.52%, FRAP: 2.87 mM FeSO₄) and α -amylase inhibitory effect (86.23%) compared to MMLP-CAM (DPPH: 49.33%, FRAP: 1.49 mM FeSO₄, α -amylase inhibition: 81.76%). These improvements are attributed to DES-induced structural modifications. Overall, this work highlights the potential of DES as a sustainable and effective medium for extracting bioactive polysaccharides with therapeutic relevance in oxidative stress and diabetes management.

Keywords: Polysaccharides, deep eutectic solvents, extraction, characterizations, oxidative stress, diabetes

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PHYTOCHEMICAL ANALYSIS AND BIOLOGICAL ACTIVITY OF *CALOPHYLLUM CANUM* HOOK F. EX T. ANDERSON: INSIGHTS INTO ANTIOXIDANT AND ANTIBACTERIAL EFFECTS AGAINST *ACINETOBACTER* *NOSOCOMIALIS* AND *ACINETOBACTER BAUMANNII*

Vivien Jong Yi Mian^{a*}, Mas Atikah Lizazman^a, Thiruvenathan Karunakaran^b,
Nor Hisam Zamakshshari^c

^aFaculty of Applied Sciences, Universiti Teknologi MARA, Kota Samarahan, Sarawak, Malaysia

^bCentre for Drug Research, Universiti Sains Malaysia, 11800 USM, Pulau Pinang, Malaysia

^cFaculty of Resource Sciences and Technology, Universiti Malaysia Sarawak, Kota Samarahan, Malaysia

*Corresponding author: vivien@uitm.edu.my

Abstract

This study investigates the phytochemical content and biological activities of extracts from the stem bark of *C. canum*, focusing on its antioxidant and antibacterial potential. Compounds were isolated from the ethyl acetate extract, revealing several known xanthenes, 1-hydroxy-7-methoxyxanthone (**1**), caloxanthone C (**2**), trapezifolixanthone (**3**), ananixanthone (**4**), euxanthone (**5**), gentisin (**6**), 2-hydroxyxanthone (**7**), α -mangostin (**9**), and a novel compound named canumolactone (**8**). The extraction process utilized sequential maceration techniques with various solvents, including *n*-hexane, dichloromethane, chloroform, ethyl acetate, and methanol, to assess the total phenolic content (TPC) and total flavonoid content (TFC). The TPC ranged from 83 to 277 mg GAE/g extract, with the ethyl acetate extract exhibiting the highest concentration (277.33 mg GAE/g). The TFC varied from 11 to 139 mg QE/g extract, with the chloroform extract showing the highest content (139.56 mg QE/g). Antioxidant activity was evaluated using the DPPH radical scavenging assay, where the ethyl acetate extract demonstrated the strongest activity with an IC₅₀ value of 7.52 μ g/mL. A strong negative correlation ($r = -0.968$) was observed between TPC and DPPH activity, indicating that higher phenolic content is associated with enhanced antioxidant activity. The antibacterial efficacy of the extracts was assessed against *Acinetobacter baumannii*, with the ethyl acetate extract showing significant activity, with minimum inhibitory concentration (MIC) values as low as 0.056 mg/mL. These findings underscore the importance of solvent choice in extracting bioactive compounds and highlight the potential of *C. canum* extracts as valuable sources of natural antioxidants and antibacterial agents.

Keywords: *Calophyllum canum*, extract, xanthenes, antioxidant, *Acinobacter baumannii*.

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PHYTOCHEMICALS AS BIOPESTICIDES FOR SAFER PEST MANAGEMENT AND HEALTHIER ECOSYSTEMS

Susanne K. Wiedmer^{a*}, Rahim Ullah^a, Tehreem Ashraf^b, Kari Hartonen^a

^aDepartment of Chemistry, University of Helsinki, Finland

^bNational center of Bioinformatic, Quaid-i-Azam University Islamabad, Pakistan

Corresponding author: susanne.wiedmer@helsinki.fi

Abstract

The increase in environmental and health issues related to synthetic pesticides emphasize the urgent need for sustainable pest management solutions through ecofriendly methods. Plants offer eco-friendly alternatives with their rich chemical diversity of secondary metabolites to target various crop pathogens with precision and minimal ecological disruption. We have studied phytochemicals of agriculture weed plants for biopesticidal potential through an integrative approach combining extraction, characterization, and molecular docking. We have analyzed the samples of different weed plants such as *Calotropis gigantea*, *Datura alba*, *Cleome gynandra*, and *Chenopodium ambrosioides*. Key phytochemicals, including β -damascenone, carvacrol, o-thymol, cis- β -elemene, and β -eudesmol have been identified in these plants, which have been further screened for their binding affinity towards acetylcholinesterase (6XYU), peptide deformylase (5CY8), and endoglucanase I (4OVW). Furthermore, pharmacokinetic studies indicate that the identified phytochemicals have drug-like properties with neither toxic nor carcinogenic effects. Our results show that the phytochemicals present in these plants have potential applications for crop pest and pathogen control. The findings contribute to the promotion of natural products by the development of biopesticides which address the dual challenges posed to human health, food security, and environmental sustainability. The discussion will address the following key areas: the extraction procedure, the phytochemical investigation conducted using gas chromatography-mass spectrometry, and the significant findings from molecular docking analysis of the compounds identified.

Keywords: biopesticides, *In silico* studies, natural product, phytochemicals, pest management, sustainable agriculture

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INVESTIGATION OF ANTI-DIABETIC POTENTIAL USING MOLECULAR SIMULATION STUDIES OF DIBENZYLIDINE-CYCLOHEXANONE CURCUMIN ANALOGS

Ranti Kamila Habibie^a, Ritmaleni^{b*}, Rumiya^b, Muchtaridi^c

^aDoctoral in Pharmaceutical Sciences, Faculty of Pharmacy, Universitas Gadjah Mada, Sleman, Yogyakarta 55281, Indonesia

^bDepartment of Pharmaceutical Chemistry, Faculty of Pharmacy, Universitas Gadjah Mada, Sleman, Yogyakarta 55281, Indonesia

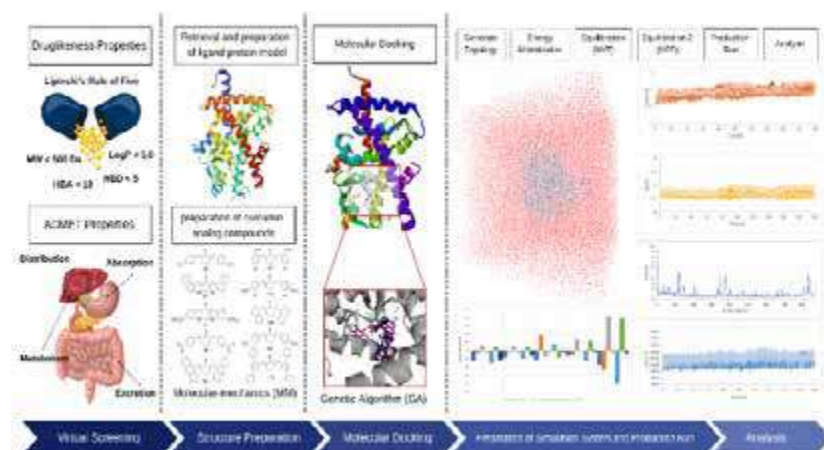
^cDepartment of Medicinal Chemistry and Analysis, Faculty of Pharmacy, Universitas Padjadjaran, Sumedang 45362, Indonesia

*Corresponding author: ritmaleni@ugm.ac.id

Abstract

Type II diabetes mellitus (T2DM) has a high prevalence in the world, in 2024 there will be around 537 million people with T2DM¹ and this number is predicted to increase yearly, one of the contributing factors is insulin resistance. PPAR γ (peroxisome proliferator-activated receptor γ) is one of the T2DM target receptors, it plays a crucial role as a control agent for adipogenesis, glucose homeostasis, and insulin sensitivity². This study aimed to investigate the antidiabetic potential of dibenzylidene-cyclohexanone curcumin analog compounds as agonist PPAR γ using *in-silico* methods. Virtual screening (including drug-likeness and ADMET properties), molecular docking (MD), and molecular dynamics simulation (MDS) were carried out using ADMETlab 3.0, Autodock 4.2, and Gromacs 2023. This research used ten compounds of curcumin analogs with each unique structure and crystal structure of PPAR γ in complex with rosiglitazone (7AWC) for analysis. All curcumin analog compounds were predicted to have good druglikeness properties, except the A119. ADME-Tox properties showed curcumin analogs are still within the limits for each parameter, but they are still fairly safe and non-toxic. The MD results showed that A117, A116, and A109 might possess a promising activator potential with binding energy -11.30; -10.83; and -10.44 kcal/mol, which is lower than the lead compound, curcumin, and the well-known activator PPAR γ , rosiglitazone, with -8.64 and -9.86 kcal/mol. The investigation continues to MDS, it showed good docked complexes flexibility, deformability, and stability proven by RMSD, RMSF, Rg, SASA, Hbond, and also MM-PBSA that did not fluctuate significantly. In conclusion, this study revealed a new potential anti-diabetes compound that activates PPAR γ to treat type 2 diabetes mellitus.

Keywords: Curcumin analogs, PPAR γ , molecular docking, antidiabetic, *in-silico*



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SILICA AGGRAVATES PULMONARY FIBROSIS THROUGH DISRUPTING LUNG MICROBIOTA AND AMINO ACID METABOLITES

Chuanyi Huo^a, Lin Tian^{a*}

^aCapital Medical University

*Corresponding author: tianlin@ccmu.edu.cn

Abstract

Silicosis, recognized as a severe global public health issue, is an irreversible pulmonary fibrosis caused by the long-term inhalation of silica particles. Given the intricate pathogenesis of silicosis, there is no effective intervention measure, which poses a severe threat to public health. Our previous study reported that dysbiosis of lung microbiota is associated with the development of pulmonary fibrosis, potentially involving the lipopolysaccharides/toll-like receptor 4 pathway¹. Similarly, the process of pulmonary fibrosis is accompanied by alterations in metabolic pathways². This study employed a combined approach of 16S rDNA sequencing and metabolomic analysis to investigate further the role of lung microbiota in silicosis delving deeper into the potential pathogenesis of silicosis. Silica exposure can lead to dysbiosis of the lung microbiota and the occurrence of pulmonary fibrosis, which was alleviated by a combination antibiotic intervention. Additionally, significant metabolic disturbances were found in silicosis, involving 85 differential metabolites among the three groups, which are mainly focused on amino acid metabolic pathways. Spearman's analysis revealed that the changed lung metabolites showed a substantial correlation with lung microbiota. The relative abundance of *Pseudomonas* negatively correlated with L-Aspartic acid, L-Glutamic acid, and L-Threonine levels³. These results indicate that dysbiosis in pulmonary microbiota exacerbates silica-induced fibrosis through impacts on amino acid metabolism, providing new insights into the potential mechanisms and interventions of silicosis.

Keywords: Silica, Pulmonary fibrosis, Lung microbiota, Metabolomics, Combined antibiotic administration

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NATURAL PRODUCTS AS POTENTIAL INHIBITORS OF ALK5 AGAINST IDIOPATHIC PULMONARY FIBROSIS: IN SILICO DOCKING ANALYSIS

Bandar A. Alyami^{a*}, Ahmed K. Hamdy^b, Al-Montaser Bellah H. Ali^c

^a Department of Pharmaceutical Chemistry, College of Pharmacy, Najran University, Najran, Saudi Arabia

^b Joint Research Center for Human Retrovirus Infection, Kumamoto University, Kumamoto, Japan

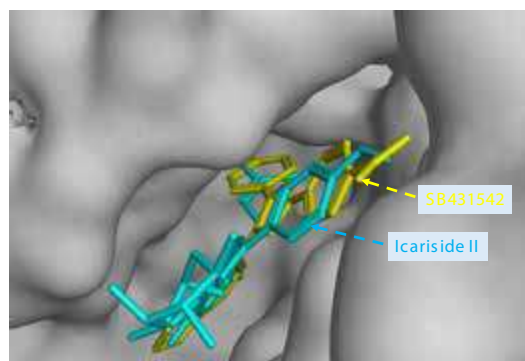
^c Department of Pharmaceutical Analytical Chemistry, Assiut University, Assiut, Egypt

*Corresponding author: baaalyami@nu.edu.sa

Abstract

Idiopathic pulmonary fibrosis (IPF) is a chronic lung disease with poor prognosis and excessive fibrosis. Existing drugs, such as pirfenidone and nintedanib, slow progression but do not stop the disease. In addition, no ALK5 inhibitors have been approved by the FDA, even though ALK5 is critical for TGF- β signaling and fibrogenesis. Identification of new ALK5 inhibitors may lead to a more efficient therapeutic option for IPF. In this study molecular docking was utilized to screen 100 natural products with diverse chemical structures to identify potential lead ALK5 inhibitors for the treatment of IPF. Molecular Docking analysis of natural products into the ALK5-binding site (PDB: 3TQM), co-crystallized with SB431542, were performed using MOE software. Binding affinity was calculated and interaction with the key residues were analyzed. The drug-likeness of the best compounds was analyzed based on the ADMET properties. Icariside II bound strongly (-9.1378 kcal/mol) and formed same critical interactions as SB431542 (-8.4943 kcal/mol). The top five strongest binding values were Icarin, Robinin, Icariside II, Dauricine and Schaftoside. A pharmacokinetic analysis identified Icariside II as the most promising candidate owing to its favorable oral bioavailability and metabolic stability. This report indicates that Icariside II is a promising ALK5 inhibitor with good pharmacokinetics that merit further optimization and experimental validation for the treatment of IPF.

Keywords: in silico docking, ALK5 inhibitor, Natural products, Idiopathic pulmonary fibrosis, Icariside II.



Superimposition of Icariside II (cyan) and SB431542 (yellow) in the ALK5 binding site of 3TQM.

GCMS-BASED PHYTOCHEMICAL ANALYSIS OF *GLYCOSMIS PENTAPHYLLA* LEAVES: *IN-VITRO* ASSESSMENT OF ANTIDIABETIC, ANTIOXIDANT, ANTI-INFLAMMATORY, AND ANTICANCER PROPERTIES AGAINST MDAMB-231, A549, AND HEP-G-2 CANCER CELL LINES

Yahya S. Alqahtani^{a,*}

^a Department of Pharmaceutical Chemistry, College of Pharmacy, Najran University, Najran, Saudi Arabia.

*Corresponding author: ysalmuneef@nu.edu.sa

Abstract

Bioactive compounds identified in various plant species from throughout the world are increasingly emerging as potential medicinal strategies. A GCMS-based phytochemical analysis of *Glycosmis pentaphylla* leaves unveiled its therapeutic potential. The study encompassed an in-vitro assessment of its antidiabetic, anti-inflammatory, antioxidants and cytotoxicity toward cancerous cell lines, breast cancer-MDAMB-231, Lung cancer-A549, and liver cancer-HEP-G-2. The results demonstrated significant therapeutic promise, including anticancer, antioxidant, wound healing, and anti-inflammatory effects. Additionally, the analysis revealed the presence of polyphenols and flavonoids, compounds known for their health-promoting properties. This research sheds light on the multifaceted medicinal properties of *Glycosmis pentaphylla* leaves, making them a promising candidate for further exploration in the field of complementary and alternative medicine.

Keywords: *Glycosmis pentaphylla*; cytotoxic; GCMS; antidiabetic, antioxidant, anti-inflammatory, wound healing

SYNTHESIS OF THE CHROMONE-THIOSEMICARBAZONE SCAFFOLD AS PROMISING α -GLUCOSIDASE INHIBITORS: AN IN VITRO AND IN SILICO APPROACH TOWARD ANTIDIABETIC DRUG DESIGN

Rima D. Alharthy^{a*}

^aChemistry Department, Science and Arts College in Rabigh, King Abdulaziz University, Jeddah, Saudi Arabia.

*Corresponding author: iaaalharte@kau.edu.sa

Abstract

Diabetes is a serious metabolic disorder affecting individuals of all age groups and prevails globally due to the failure of previous treatments. This study aims to address the most prevalent form of type 2 diabetes mellitus (T2DM) by reporting on the design, synthesis, and in vitro as well as in silico evaluation of chromone-based thiosemicarbazones as potential α -glucosidase inhibitors. Hybrids of these two compounds were synthesized to improve antidiabetic properties. A novel category of fluorosubstituted chromone-thiosemicarbazones was evaluated for their in vitro α -glucosidase inhibition activities. Sixteen compounds were synthesized by attaching different groups, and their SAR analysis revealed that a simple methyl group on the nitrogen atom produced an exceptional lead compound. Additionally, phenyl and aryl derivatives exhibited comparable activity, whereas the activity of all the derivatives surpassed that of acarbose. In vitro experiments showed that the tested compounds were significantly more potent than the standard acarbose, with the lead compound 3n exhibiting an IC_{50} value of $0.40 \pm 0.02 \mu\text{M}$, ~2183-fold higher than acarbose having an IC_{50} of $873.34 \pm 1.67 \mu\text{M}$. A kinetic mechanism analysis demonstrated that compound 3n exhibited reversible inhibition of α -glucosidase. To gain deeper insights, in silico molecular docking, pharmacokinetics, and molecular dynamics simulations were conducted for the investigation of the interactions, orientation, stability, and conformation of the synthesized compounds within the active pocket of α -glucosidase.

Keywords: antidiabetic, chromone, molecular dynamic simulations, thiosemicarbazone, α -glucosidase

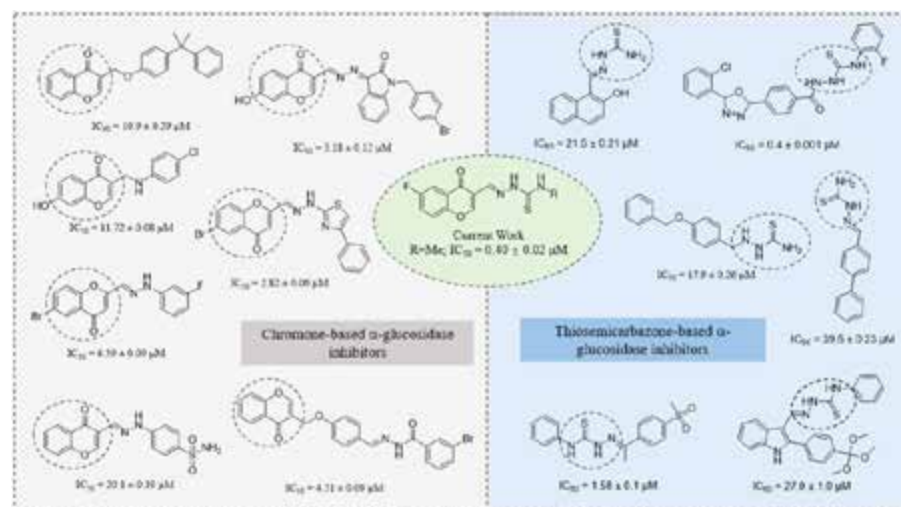


Figure 1. Some derivatives based on chromone and thiosemicarbazone possess α -glucosidase inhibitory activity.

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SYNTHESIS, ANTIMICROBIAL AND ANTIOXIDANT EVALUATION WITH *IN SILICO* STUDIES OF NEW THIAZOLE SCHIFF BASE DERIVATIVES

Md. Shahazada Shah ^a, Mohammad Mostafizur Rahman ^{a*}, Md. Din Islam ^b, Abdullah Al-Macktuf ^a, Junaid Uddin Ahmed ^c, Hiroshi Nishino ^d, Md. Aminul Haque ^{a*}

^a Department of Chemistry, Jagannath University, Dhaka 1100, Bangladesh

^b Department of Chemistry, Chittagong University of Engineering & Technology, Chattogram 4349, Bangladesh

^c Department of Chemistry, Khulna University of Engineering & Technology, Khulna 9203, Bangladesh

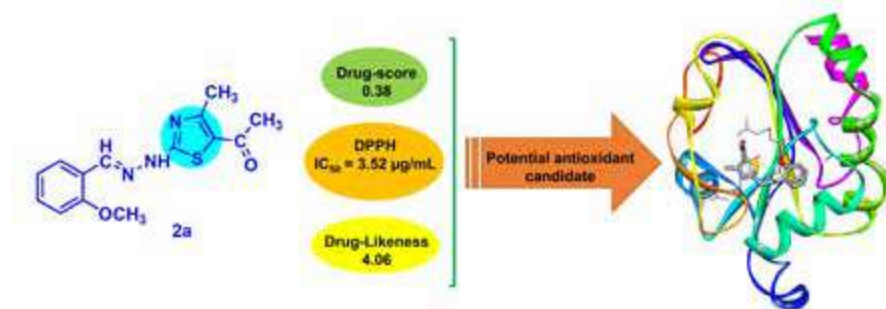
^d Department of Chemistry, Graduate School of Science and Technology, Kumamoto University, Kumamoto, Japan

*Corresponding author: amin2k12@chem.jnu.ac.bd

Abstract

A series of nineteen thiazole Schiff base derivatives 2a-2s were synthesized and elucidated by spectral analyses (IR, ¹H NMR and HRMS). The evaluation of their antimicrobial activities against two gram-positive, two gram-negative, and two fungal strains revealed that some compounds displayed moderate antimicrobial activities compared to standard ciprofloxacin and miconazole in disc diffusion technique. Compound 2a displayed very strong antioxidant efficacy ($IC_{50} = 3.52 \pm 0.86 \mu\text{g/mL}$) compared to standard ascorbic acid ($IC_{50} = 27.34 \pm 1.86 \mu\text{g/mL}$) in DPPH free radical scavenging assay. Compounds 2j, 2k, and 2m displayed significant antioxidant activities in this assay as well. *In silico* analysis predicted that the synthesized compounds follow the Lipinski's rule of five and Veber's rule with one exception. The compounds displayed good drug-likeness and drug-score properties. The molecular docking studies predicted that the synthesized thiazole Schiff base derivatives are tolerable in putative receptor binding sites.

Keywords: Thiazole, Antimicrobial activities, Antioxidant activities, ADME, Molecular docking



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SYNTHESIS, ANTIMICROBIAL EVALUATION, ADMET PREDICTION, MOLECULAR DOCKING AND DYNAMICS STUDIES OF PYRIDINE AND THIOPHENE MOIETIES CONTAINING CHALCONES

Fahmida Akhter^a, Sumita Saznin Marufa^a, S M Anyet Ullah Shohag^b, Hiroshi Nishino^c, Mohammad Sayed Alam^a, Md. Aminul Haque^a, Mohammad Mostafizur Rahman^{a*}

^aDepartment of Chemistry, Jagannath University, Dhaka 1100, Bangladesh.

^bDepartment of Chemical Engineering and Polymer Science, Shahjalal University of Science and Technology, Sylhet 3114, Bangladesh.

^cDepartment of Chemistry, Graduate School of Science and Technology, Kumamoto University, Kumamoto, Japan

*Corresponding author: mostafiz@chem.jnu.ac.bd

Abstract

Microbial resistance to various antimicrobial agents has become a serious challenge in the healthcare sector within the last few decades around the globe.¹ Thus, it is a pressing need to discover and develop potential antimicrobial agents along with efficient synthesis procedure. Chalcones and its derivatives secured a significant attention with their multifaceted activities and simple synthesis procedure in the field of medicinal chemistry.² In this study, three pyridine and four thiophene containing chalcone derivatives were synthesized *via* Claisen-Schmidt condensation reaction. Different spectral analyses (IR, ¹H NMR, HRMS) clarified the structures and these proposed compounds were screened for antimicrobial activity by agar disk diffusion technique. Compound **1c** was conspicuously active against most of the bacterial and fungal strains. It displayed higher activity against *B. cereus* (22.3 ± 0.6 mm), *S. sonnei* (43.3 ± 0.6 mm) and *S. boydii* (34.0 ± 1.0 mm) compared to the standard ceftriaxone (20.3 ± 0.6 mm, 40.3 ± 0.6 mm and 25.7 ± 0.6 mm, respectively). In addition, the exhibited inhibition zone of compound **1c** against all fungal strains was higher than the standard amphotericin B. All the newly synthesized derivatives satisfied the ADME properties, and no toxicological risks were found. All compounds were docked against three protein receptors with the range of binding affinity of -6.3 to -9.6 kcal/mol. Molecular dynamics simulation was scrutinized further for compound **1c** in three protein-ligand complexes where RMSD and RMSF data were below 2 Å, proposing its stability inside and minimal structural changes.

Keywords: Chalcone, Antimicrobial activities, ADMET, Docking, Molecular dynamics



1. Synthesis of chalcone derivatives containing pyridine and thiophene moieties, respectively.

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EVALUATION OF THE ANTI-HIV AND ANTI-DENV ACTIVITIES OF SOME TRIAZENES

Seynabou SOKHNA^{a, b, c}, Natacha Mérindol^e, Marie-Pierre Girard^e, Insa SECK^a, Samba Fama NDOYE^a, Issa SAMB^b, Marc PRESSET^c, Erwan LE GALL^c, Lionel BERTHOUX^d, Isabel DESGAGNÉ-PENIX^e, Matar SECK

^{a2}*Laboratoire de Chimie Organique et Thérapeutique, Faculté de Médecine, de Pharmacie et d'Odontologie de l'Université Cheikh Anta Diop de Dakar, BP 5005 Dakar-Fann, Sénégal;*

Laboratoire de Chimie de Coordination Organique (LCCO), Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop de Dakar, Dakar, Sénégal.

^b *Organic and Therapeutic Chemistry Research Team (ECOT), Alioune Diop University of Bambey, Senegal*

^c *UMR 7182 - ICMPE - Institute of Chemistry and Materials Paris Est, Thiais-France*

^d *Dept. of Chemistry, Biochemistry and Physics, UQTR, Trois-Rivières, QC, Canada*

^e *Dept. of Biomedical Sciences, UQTR, Trois-Rivières, QC, Canada*

Abstract

Human immunodeficiency virus (HIV) and dengue virus (DENV) are RNA viruses, like influenza and coronavirus. With more than 100 million cases of dengue fever annually ⁽¹⁾ and 39.9 million people living with HIV in 2023⁽²⁾, they constitute a major public health problem, particularly in Africa. In the absence of specific treatment for dengue and AIDS, existing drugs aim to keep infected people healthy, and significant resistance to antiretrovirals has been observed, making their treatment difficult. Thus, access to new antivirals with few side effects is a major challenge. Triazenes, a class with three successive nitrogen atoms ⁽³⁾, widely studied for their anticancer properties ^(4,5), are attracting increasing interest for their antiviral potential ⁽⁶⁾.

This study aims to access to triazenes by diazocopulation, evaluate their activity against DENV and HIV at concentrations between 1 and 100 μ M and finely measure their cytotoxicity by flow cytometry on THP-1 and HUH-7 cells.

A library of 54 triazenes was obtained, 40 in aqueous medium and 14 in organic medium, with yields ranging from 13 to 97%. Interesting anti-DENV activity was observed for compounds **14** and **28**, with EC₅₀ values of 8.08 μ M and 7.8 μ M respectively, as well as low cytotoxicity with CC₅₀ values of 75.63 and 100 μ M respectively and good selectivity indices (9.36 and 12.8). Satisfactory results were obtained for anti-HIV activity: compounds **37**; **41** and **53**, with EC₅₀ values of 9.1; 11.8 and 13.7 μ M respectively, showed low cytotoxicity and low percentages of necrotic cells (PI+) of 4.76%; 3.93% and 11.7%.

These preliminary results pave the way for targeted structural optimization and a better understanding of triazene-virus interactions. They highlight the potential of triazenes as candidates for the development of new antiviral therapies, particularly in the context of dengue/HIV coinfection or resistance to current treatments.

Keywords: triazene, anti-HIV, anti-DENV.

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CHEMICAL PROFILING AND QUANTIFICATION OF SELECTED ANTHRAQUINONES FROM THE ROOTS EXTRACTS OF *RENNELIA BORNEENSIS* BAILL

Nurunajah Ab Ghani^{1,2*}, Nur Afiqah Nadhiah Ammar Rushdan^{1,2}, Nurufazlina Edayah Rasol^{1,2}, Wan Mohd Nuzul Hakimi W Salleh³, Adlin Afzan⁴, Monica Suleiman⁵

¹Atta-ur-Rahman Institute for Natural Product Discovery, Universiti Teknologi MARA, 42300 Bandar Puncak Alam, Selangor, Malaysia

²Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia

³Department of Chemistry, Faculty of Science and Mathematics, Universiti Pendidikan Sultan Idris, Tanjong Malim, Perak, Malaysia

⁴Herbal Medicine Research Centre, Institute for Medical Research, National Institutes of Health, Ministry of Health Malaysia, Setia Alam, 40170 Shah Alam, Malaysia

⁵Institute for Tropical Biology & Conservation, University Malaysia Sabah, 88400 Kota Kinabalu, Sabah, Malaysia

*Corresponding author: nurunajah@uitm.edu.my

Abstract

Rennellia borneensis Baill. (Rubiaceae), commonly known as Borneo ginseng, is an endemic plant species of Sabah, particularly found in the Imbak Canyon Conservation Area (ICCA). Its roots have been traditionally used for medicinal purposes, including the treatment of cancer, poisoning, aging-related ailments, and for enhancing vitality and energy. Despite its traditional significance, limited scientific research has been conducted on its secondary metabolites and biological properties. Understanding its chemical profile is crucial for validating traditional uses and ensuring sustainable utilization. This study provides the first systematic analysis of the secondary metabolites in the dichloromethane root extract of *R. borneensis*. High-resolution mass spectrometry, combined with a data-dependent acquisition (DDA) LC-MS/MS approach, identified 17 compounds, including anthraquinones, flavonoids, isoflavonoids, and triterpenoids. The LC-MS phytochemical profile was further confirmed by the isolation of two anthraquinones, rubiadin and 3-hydroxy-2-methyl-9,10-anthraquinone, which were used as standards for quantification. A validated HPLC assay determined their concentrations in the extract to be 1.21 µg/g and 4.41 µg/g, respectively. These findings suggest that *R. borneensis* is a promising herbal medicine, particularly due to its abundance of anthraquinones, which may contribute to its biological activity. Furthermore, the developed analytical method is applicable to low-yield samples, supporting environmentally sustainable research and utilization.

Keywords: *Rennellia borneensis*; Dereplication; Quantification; Anthraquinone; SIRIUS, GNPS

SYNTHESIS AND BIOLOGICAL EVALUATION OF NOVEL COUMARIN DERIVATIVES BEARING SULFONAMIDE MOIETY AS POTENT α -GLUCOSIDASE INHIBITORS

Syahrul Imran^{a,b*}, Alim Alsukor^{a,b}, & Nurul Alam Inayatsyah^{a,b}

^aAtta-Ur-Rahman Institute for Natural Product Discovery, Universiti Teknologi MARA (UiTM), Puncak Alam Campus, 42300, Bandar Puncak Alam, Selangor, Malaysia

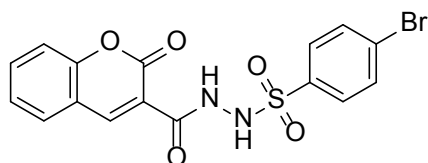
^bFaculty of Applied Science UiTM, 40450, Shah Alam, Selangor, Malaysia

*Corresponding author: syahrulimran@uitm.edu.my

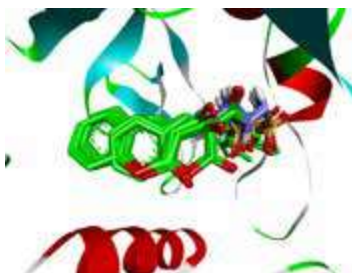
Abstract

Acarbose, miglitol and voglibose are α -glucosidase enzyme inhibitors that are clinically used to treat type-II diabetes mellitus. However, they are also associated with several adverse side effects. In this study, a series of sulfonamide-substituted coumarin was synthesized in a three-step reaction from precursor, 2-oxo-2H-chromene-3-carboxylic acid. The structure of all synthesized compounds was confirmed using NMR, FTIR and LCMS analysis and found to be in good agreement with the calculated values. Synthesized coumarin derivatives were screened for their in vitro α -glucosidase inhibitory activity. Besides compound **8**, **15** compounds demonstrated good to excellent inhibitory activity with the IC_{50} values ranging from 40.6 to 2021 μ M as compared to acarbose ($IC_{50} = 3410 \pm 1.54$ μ M). A structure–activity relationship was established to form correlation of the substituents effect with inhibitory activity. It was found that chlorine substituent played an important role in the activity compared to other halogen substituents. Derivatives showing inhibition activity were subjected to docking studies to identify the binding modes contributing towards the inhibition activity.

Keywords: Coumarin, Sulfonamide, α -Glucosidase, Enzyme inhibition, Anti-diabetic agent



Compound 8



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EXPLORING THE NATURAL PRODUCT OF THERAPEUTIC POTENTIAL OF KAFFIR LIME FROM THE INSIGHTS OF LC-MS ORBITRAP ANALYSIS PERSPECTIVE

Kathleen J. Jalani^{a,*}, Fatimah Salim^{a,b}, Nurulfazlina Edayah Rasol^{a,b}, Adiez Sapura Azmi^b

^aAtta-ur-Rahman Institute for Natural Product Discovery (AuRIns), Universiti Teknologi MARA Selangor Branch, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor, Malaysia

^bFaculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia

*kathleen@uitm.edu.my

Abstract

Kaffir lime (*Citrus hystrix* DC) has long been valued in traditional medicine for its diverse therapeutic properties, including antioxidant, anti-inflammatory, antibacterial, and hepatoprotective effects. This plant is rich in bioactive compounds such as flavonoids, terpenoids, and essential oils, which are believed to promote healing, reduce inflammation, and support overall recovery. Recent advances in analytical chemistry, particularly the application of high-resolution Liquid Chromatography-Mass Spectrometry (LC-MS) Orbitrap technology, has enabled comprehensive profiling of the bioactive compounds responsible for these health benefits. The present study has provided detailed profiles of Kaffir lime's chemical constituents, revealing several key bioactive compounds including flavonoids (quercetin, kaempferol, keracyanin, rihofolin, cynaroside, neodiosmin, and rutin), and alkaloids (adenosine and the amino acids (D-(+)-poline and pipercolic acid). Keracyanin was reported for the first time in the ethanolic kaffir lime extract. These compounds were identified and quantified with high accuracy and resolution, offering insights into their potential pharmacological activities. The LC-MS results showed significant concentrations of compounds linked to antioxidant and anti-inflammatory effects, which may contribute to the plant's ability to support good health and well-being. The antioxidant assay revealed that kaffir lime extract exhibited 80.45 % DPPH radical scavenging activity, approaching the efficacy of the standard antioxidant control, ascorbic acid (89.81 %). Notably, kaffir lime demonstrated nearly 1.4 times higher activity as compared to commercialized natural antioxidant such as green tea (58.05 %). Therefore, Kaffir lime extract highlighting its superior alternative natural antioxidant potential. These findings emphasize the value of Kaffir lime as a natural therapeutic agent and highlight the importance of advanced analytical techniques like LC-MS technology in identifying bioactive compounds for potential applications. Future research should explore the molecular mechanisms behind these effects and their synergistic potential human health.

Keywords: Natural product, kaffir lime, LCMS Orbitrap

STILBENES FROM *HOPEA FERREA* OF LIMESTONE FORESTS: A PROMISING SOURCE OF ANTIBIOFILM AGENTS

Nurul 'Izzah Mohd Sarmin^{a,b*}, Mohd Fithrie Lali @Zailani^{a,c}, Isna Athirah Othman^{a,c},
Fatimah Salim^{a,c},

^aAtta-ur-Rahman Institute for Natural Product Discovery, Level 9, Universiti Teknologi MARA,
Puncak Alam Campus 42300, Bandar Puncak Alam, Selangor:

^bCentre of Preclinical Science Studies, Faculty of Dentistry, Universiti Teknologi MARA, Sungai Buloh Campus
47000 Sungai Buloh, Selangor:

^cFaculty of Applied Science, Universiti Teknologi MARA, 40450 Shah Alam, Selangor.

*Corresponding author: izzahsarmin@uitm.edu.my

Abstract

Biofilm formation by *Streptococcus mutans* is a key virulence factor in the development of dental caries, enabling persistent colonization of tooth surfaces and resistance to antimicrobial treatments. In the ongoing search for novel biofilm inhibitors from natural sources, this study investigates the antibiofilm potential of stilbenes isolated from *Hopea ferrea*, a medicinal tree native to limestone forest ecosystems. Plant material from *H. ferrea* was collected from a limestone forest in Pulau Tuba, Langkawi, Malaysia and subjected to solvent extraction and chromatographic separation to isolate stilbene compounds. The chemical structures of isolated compounds were elucidated using NMR and LC-MS techniques. Antibiofilm activity against *S. mutans* was assessed using a crystal violet microtiter plate assay to quantify biofilm biomass. Additionally, minimum inhibitory concentration (MIC) and minimum biofilm inhibitory concentration (MBIC) values were determined to evaluate crude extracts selectivity. Two stilbenes were successfully isolated and characterized as α -viniferin and ampelopsin A. All compounds demonstrated concentration-dependent inhibition of *S. mutans* biofilm formation. Notably, biofilm disruption occurred without significant inhibition of planktonic growth, suggesting a mechanism targeting adhesion or extracellular matrix production. Stilbenes derived from *Hopea ferrea* exhibit promising antibiofilm activity against *S. mutans*, highlighting their potential as lead compounds for the development of alternative strategies to manage biofilm-related oral diseases. Further mechanistic studies and in vivo evaluation are warranted to advance these findings toward therapeutic applications.

Keywords: *Hopea ferrea*; antibiofilm; stilbene; *Streptococcus mutans*; limestone forest

CHEMICAL PROFILING AND ANTIMICROBIAL EVALUATION OF SECONDARY METABOLITES FROM ARCTIC FUNGI INDUCED BY EPIGENETIC MODIFIERS

Siti Hajar Sadiran^{a,b,*}, Siti Aisah Alias^c, Jean-Frédéric F. Weber^d

^aAtta-ur-Rahman Institute for Natural Product Discovery, Universiti Teknologi MARA Selangor, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor, Malaysia.

^bSchool of Biology, Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia.

^cInstitute of Ocean and Earth Sciences, and National Antarctic Research Centre, University of Malaya, 50603 Kuala Lumpur, Wilayah Persekutuan, Malaysia.

^dLaboratoire de Pharmacognosie, UFR Sciences Pharmaceutiques, Université de Bordeaux, 146 rue Léo Saignat, 33076 Bordeaux cedex, France.

*Corresponding author: hajarsadiran@uitm.edu.my

Abstract

Secondary metabolite production in fungi can be modulated through various approaches, including culture-dependent techniques, the use of epigenetic modifiers, and genomic-based strategies. In this study, fungal secondary metabolite production was explored in the presence of epigenetic modifiers using a microscale fermentation approach. Arctic fungus, *Pleosporales* sp. and *Penicillium samsonianum* were isolated from soil samples collected in Longyearbyen, Svalbard Island, Norway. These fungi were fermented in 96-deep well microtiter plates with potato dextrose broth (PDB) supplemented with epigenetic modifiers namely suberoylanilide hydroxamic acid (SAHA) and S-adenosylhomocysteine (SAHC), 5-azacytidine (5-AC), valproic acid (VA) and sodium butyrate (SB), along with a control (PDB without any epigenetic modifiers). The fungal cultures were extracted via solid-phase extraction, and the crude extracts were analysed by high-performance liquid chromatography (HPLC). The antimicrobial activity of the crude extracts was evaluated against *Enterococcus faecium* (ATCC 51858), *Staphylococcus aureus* (ATCC 25923), *Pseudomonas aeruginosa* (ATCC 27853) and *Escherichia coli* (ATCC 25922) using the MTT assay. Both *Pleosporales* sp. and *P. samsonianum* produced crude extracts exhibiting antimicrobial activity against all tested microorganisms. HPLC analysis showed that SAHA and SAHC enhanced the production of secondary metabolites in the tested fungi. Chemical structures of the isolated compounds were determined based on spectroscopic methods, including MS, NMR, and UV/Vis. Two major secondary metabolites were identified: curvulin from *Pleosporales* sp. and 2,3-dihydro-2,2,4-dimethyl hydroxy-5-*trans* propenylfuran-3-one from *P. samsonianum*. This finding highlights the potential of epigenetic modifiers in enhancing fungal secondary metabolite production.

Keywords: Arctic fungi, epigenetic modulation, *Penicillium samsonianum*, *Pleosporales* sp.

LC-MS/MS-DRIVEN COMPOUND ANNOTATION AND ISOLATION FROM MALAYSIAN *UNCARIA* SPECIES

Nursyaza Husna Shaharuddin^a, Adlin Afzan^b, Rohaya Ahmad^a, Fatimah Salim^{a,c*}

^aFaculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor Darul Ehsan

^bHerbal Medicine Research Centre, Institute for Medical Research, National Institutes of Health, Setia Alam, 40170 Shah Alam, Selangor, Malaysia

^cAtta-ur-Rahman Institute for Natural Product Discovery (AuRIns), Universiti Teknologi MARA Selangor Branch, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor Darul Ehsan, Malaysia

*Corresponding author: fatimah2940@uitm.edu.my

Abstract

The *Uncaria* genus (Rubiaceae), consisting of 34 known species worldwide, has been traditionally used to treat a variety of ailments. Fourteen of these species are found in Malaysia and hold significant potential for the discovery and development of new pharmaceuticals. However, compared to the extensively studied *Uncaria tomentosa* from Peru and *Uncaria guianensis* from China, Malaysian *Uncaria* species remain relatively underexplored in terms of phytochemistry and biological activity. Previous investigations on Malaysian *Uncaria* have yielded over 20 identified compounds, some with promising bioactivities. A major challenge, however, is the repeated isolation of known compounds across different species, which limits novelty in drug discovery. To address this, a dereplication approach using LC-MS was employed to chemically profile leaf and stem extracts from seven Malaysian *Uncaria* species, namely *U. lanosa* var. *ferrea*, *U. cordata* var. *cordata*, *U. cordata* var. *ferruginea*, *U. longiflora* var. *pteropoda*, *U. gambir*, *U. tomentosa*, and *U. acida*, resulting in a total of 14 samples analyzed. LC-ESI-MS data interpretation through MZmine and SIRIUS facilitated the annotation of 98 compounds via spectral library matching and 387 compounds via SIRIUS (116 by class, 271 by name). The stem extract of *U. lanosa* var. *ferrea* was found to be chemically distinct and selected for targeted compound isolation. This led to the identification of two new isomeric alkaloids, structurally elucidated through advanced spectroscopic techniques as new 21-carbonyl derivatives of the pentacyclic oxindole alkaloids (POAs) isopteropodine and pteropodine. These newly discovered compounds were named 21-oxoisopteropodine and 21-oxopteropodine. The study demonstrates that LC-MS dereplication is a powerful strategy for accelerating the identification of novel compounds and enhancing chemotaxonomic resolution. This approach provides a valuable model for efficient natural product discovery and characterization in other medicinal plant species.

Keywords: *Uncaria* species, LCMS dereplication, natural product discovery, pentacyclic oxindole alkaloids, phytochemical profiling

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GENDER EQUALITY IN THE CHEMICAL SCIENCES - AN INTERSECTIONAL APPROACH

Alejandra PALERMO

Royal Society of Chemistry, Burlington House, Piccadilly London, W1J0BA, United Kingdom

Corresponding author: palermoa@rsc.org

Abstract

It is generally recognised that to get the very best scientific outputs we need a diversity of inputs and talents. However, progress is still slow and yet not well understood or actioned how to truly achieve diversity and how to ensure that those diverse inputs and talents are included, accepted, valued and empowered. Current evidence shows that a continued challenge for gender equality exists, particularly in retaining and developing women into positions of leadership within the chemical sciences. Given the global nature of our discipline and the scale of the issues identified, there is no doubt that it is imperative to work collaboratively across the community and increase the voice and representation of the Global South. During my presentation, I will discuss the challenges and opportunities in making the chemical sciences fully inclusive and diverse. I will cover a broad range of topics including creating a global inclusive research culture, and challenging the traditional measures of career success, and, hopefully, identify next steps together.

Keywords: Inclusion, Diversity, Equality, Gender, Intersectionality

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3. A vision for science culture

SUPPORTING AND INCREASING THE VISIBILITY OF WOMEN IN SCIENCE

Frances Separovic^{a,*}

^a*School of Chemistry, Bio21 Institute, University of Melbourne, VIC 3010, Australia*

^{*}*Corresponding author: fs@unimelb.edu.au*

Abstract

Attracting women and girls to science, technology, engineering and mathematics (STEM) and providing an environment for them to thrive and progress is a shared responsibility of government, academia, the education system, industry, and the community. I will discuss the Women in STEM Decadal Plan¹, developed by the Australian Academy of Science (AAS) in collaboration with the Australian Academy of Technology & Engineering. This ten-year plan offers a vision and opportunities to guide stakeholders as they identify and implement specific actions needed to build the strongest STEM workforce to support Australia. The AAS also hosts the STEM Women website^{2a}, an online directory which aims to promote gender equity in STEM by showcasing the breadth of scientific talent to enable a diverse range of women to be offered opportunities to progress their careers and personal capabilities. In partnership with the Association of Academies & Societies of Sciences in Asia (AASSA) and the InterAcademy Partnership (IAP) in September 2021 this was extended to STEM Women Asia^{2b} to help discover the diversity of women with STEM skills across Asia and Oceania. Then in November 2022, STEM Women Global^{2c} was launched to increase the visibility of women working in STEM worldwide. Further, the AAS convenes the International Science Council (ISC) Regional Focal Point for Asia & the Pacific (RFP-AP)³, which acts as a hub for ISC members and activities in the region. The ISC RFP-AP aims to ensure that the unique needs and priorities of the Asia and Pacific regions are integrated into the global scientific dialogue. A mentoring programme⁴ commenced in September 2024 to connect early career researchers (ECRs) with senior science mentors to guide young scientists from low-income nations within the region to become future leaders in academia. A case study of an ECR in chemistry who participated in the program will be presented.

Keywords: diversity and inclusion, gender equity, SDG5, STEM women, women in science

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SHAPING THE FUTURE OF CHEMISTRY: IUPAC'S GUIDING PRINCIPLES FOR RESPONSIBLE CHEMISTRY

Javier Garcia-Martinez

Department of Inorganic Chemistry, University of Alicante, 03690, Alicante, Spain

**Corresponding author: j.garcia@ua.es*

Abstract

The International Union of Pure and Applied Chemistry (IUPAC) is undertaking a project to develop a set of Guiding Principles informed by ethics, diversity, equity, and inclusion values. By emphasizing responsible, transparent, and ethical behaviors in chemistry, this initiative seeks to engage a broad audience and foster a culture of integrity within the field. In my presentation, I will explore the critical role of chemistry in addressing global challenges through ethical innovation, sustainability, and interdisciplinary collaboration. [1] I will emphasize the responsibility of chemists to advance scientific knowledge while ensuring safety, equity, and integrity in research and practice. By fostering an inclusive and diverse community, promoting responsible data use, and enhancing public engagement, chemistry can drive transformative solutions for society and the environment. I will highlight the importance of integrating ethical considerations into scientific advancements and the need for open access to information, ultimately shaping a more sustainable and just future through chemistry. [2] Ultimately, my presentation will call for a collective effort to align chemistry with broader societal goals, reinforcing its role in shaping a more sustainable, just, and scientifically empowered future.

Keywords: Ethics, IUPAC, responsible chemistry, education, guidelines

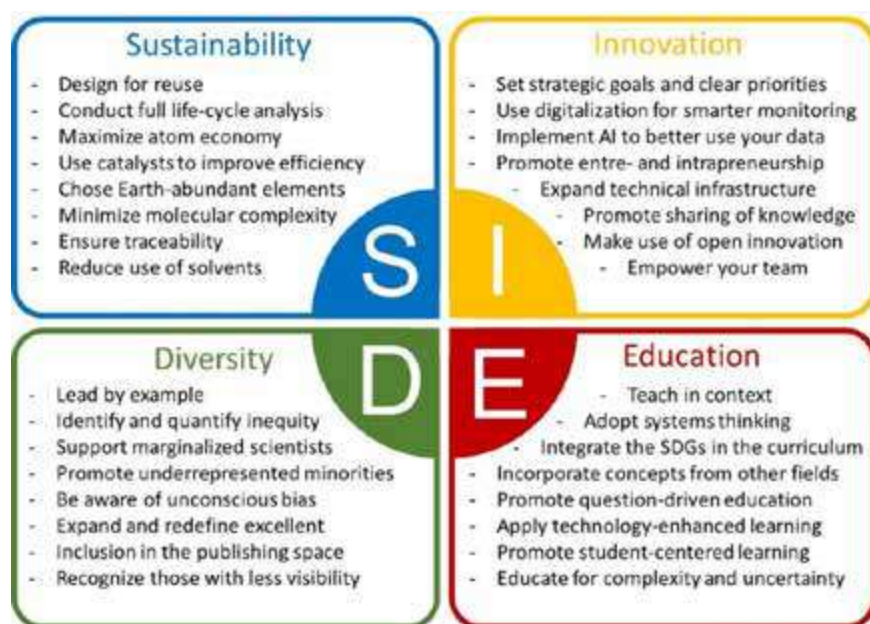


Figure 1. The SIDE vision for Chemistry 2030 comprises a number of recommendations intended to move towards a more sustainable, innovative, and inclusive chemistry. From reference [1]

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HOW TO MAKE CHEMISTRY INCLUSIVE FOR BLIND OR LOW VISION (BLV) STUDENTS: EXAMPLES FROM DIFFERENT CHEMISTRY TOPICS

Mustafa Sözbilir^{a,*}

^aAtatürk University, Kazım Karabekir Faculty of Education, Department of Mathematics and Science Education, Chemistry Education, Erzurum-Türkiye
*Corresponding author: sozbilir@atauni.edu.tr

Abstract

Science has emerged as one of the most important content areas in the core curriculum. However, traditional pedagogy is highly dependent on visual models of chemistry phenomena and chemistry instruction typically relies heavily on visual imagery and those with little or no vision have few avenues available to them to access science content and processes.

Blindness or low vision (BLV) is defined as visual impairment, which is the decreased ability to see to a degree that causes problems in education as well as in daily life. Students with visual impairment struggle with learning concepts in chemistry due to using visual representations such as figures, images, equations and graphs. However, chemistry could be made more inclusive to those students through collaboration and specific adaptation both in the classroom and laboratory by providing simple adaptations or doing some essential modifications to help them gain experience with measuring, balancing and weighing a variety of materials with simple adaptations or modifications.

In this talk, I will present examples of how they are adapted to the needs of students with BLV from different chemistry topics such as heat and temperature, heat transfer (Kızılaslan, Zorluoğlu, & Sözbilir, 2019; Kızılaslan & Sözbilir, 2020), and chemical representations (Teke & Sözbilir, 2029). The activities and materials used are based on economical and easily accessible everyday materials as well as 3D printed materials intentionally developed to the needs of BLV students. The findings showed that students' learning and motivation towards learning chemistry are enhanced.

Keywords: Inclusive chemistry education, visual impairment, blindness or low vision (BLV)

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EXPANDING GENDER EQUITY: RESULTS FROM A CROSS-NATIONAL, CROSS-SECTOR STUDY OF STEM CAREERS

Peter, T.^{a,*}, Hoang, L.^b, Dengate, J.^a, Farenhorst, A.^a, Wolfram, A.^c, & Salminen, M.^d

^a *University of Manitoba.*

^b *Western University.*

^c *RWTH Aachen University.*

^d *Uppsala University.*

*Corresponding author: tracey.peter@umanitoba.ca

Abstract

Recruiting and retaining women in STEM (Science, Technology, Engineering, and Mathematics) jobs and careers remains a pressing concern for many countries in the Global North including Canada, Sweden, and Germany. Previous research into the leaky pipeline finds that workplace incivility contributes to women exiting these fields. Yet, it is unclear which mechanisms of workplace incivility are more likely to impact turnover intention. To address this gap, we perform a mixed-methods analysis of women's experiences working in EICT jobs in Canada, Sweden, and Germany. The results of the serial mediation model analysis show significant indirect effects among incivility, perceptions of organizational equity, emotional exhaustion, and intent to leave. This suggests that women who experience increased levels of incivility and/or hostility in the workplace are less likely to perceive their organization as equitable; that those who do not perceive their workplace as equitable are more likely to report more emotional exhaustion; and that respondents who report elevated emotional exhaustion are more likely to indicate that they intend to leave their workplace within the next two years. A content analysis of open-ended survey responses sheds light onto various types of uncivil and hostile acts and behaviours perpetrated against respondents because of their gender. This qualitative data contextualizes the statistical findings by offering a view into the lived experiences of women working within EICT.

Keywords: Gender equity, Workplace climate, Job attrition, Organizational equity, Retention

FROM PERIODIC TO EQUAL TABLE: HARNESSING NANOCARBON TECHNOLOGY FOR A COOLER, CARBON-NEUTRAL, AND INCLUSIVE WORLD

Rozzeta Dolah^{a*}

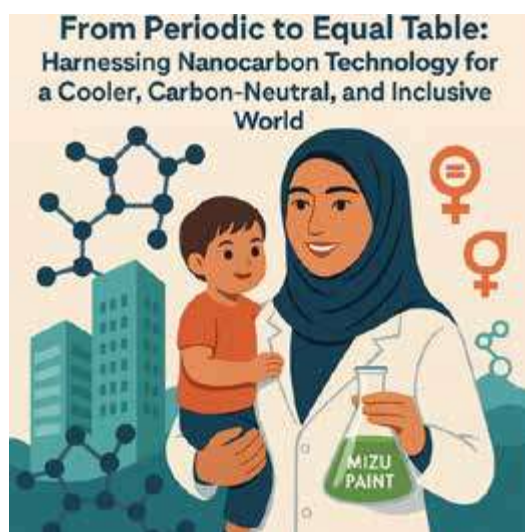
Faculty of Artificial Intelligence, Level 5, Menara Razak, Universiti Teknologi Malaysia, Jalan Sultan Yahya Petra, 54100 Kuala Lumpur, Malaysia

**Corresponding author: rozzeta.kl@utm.my*

Abstract

The Periodic Table is the foundation of chemistry, but in today's world, the vision beyond elements to address sustainability, equity, and inclusivity must be expanded. Chemistry is about shaping the future, and that future must be one that is climate-resilient, sustainable, and gender-inclusive. As a woman technopreneur, scientist, lecturer, and a mother, advancing green nanotechnology is not just about mitigating climate change—it is about creating a world where opportunities, innovations, and leadership in science are accessible to all, regardless of gender. This talk explores how nanocarbon-based functional coatings, such as **MIZU Paint**, can contribute to a cooler, carbon-neutral future while also empowering women in science and technology (STEM) to lead sustainability-driven transformations. Nanotechnology-driven solutions, such as high-performance nanocarbon coatings, provide a dual climate benefit that are 1) Urban Cooling – By reducing heat absorption, these coatings lower energy consumption, decreasing reliance on air conditioning and minimizing greenhouse gas emissions and 2) CO₂ Adsorption – By integrating nanocarbon technology, these materials actively remove carbon dioxide from the atmosphere powered by **ZetaTech™**, contributing to global decarbonization efforts. However, sustainability must also be equitable. The transition from a “Periodic Table” to an “Equal Table” symbolizes not only the need for cleaner technologies but also the necessity of gender-inclusive leadership in chemistry and innovation. Sustainable Development Goal 5 (SDG 5: Gender Equality) calls for equal access to opportunities in STEM fields, yet women remain underrepresented in many scientific and entrepreneurial spaces. From scientific research to business leadership, trailblazing insights into how gender equity can accelerate climate action, foster inclusive technological advancements, and inspire the next generation of women scientists and technopreneurs are shared. The journey reflects a broader intersection of science, entrepreneurship, and gender equity, reinforcing the message that chemistry is not just about the elements—it is about the people who shape its future.

Keywords: Periodic Table, STEM, Nano technopreneur, cooling paint, CO₂ adsorbent coating



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NOT JUST AT THE TABLE: LEADING SCIENCE BY REDEFINING WHO THRIVES

Josephine Tsang

Executive Director, Chemical Institute of Canada

**Corresponding author: jtsang@cheminst.ca*

Abstract

The future of science demands more than research excellence, it calls for a transformation in who participates, who leads, and how success is defined. While gender equality, achieved through equal access and opportunity, is a vital first step, true transformation in science begins with gender equity: redesigning the systems, cultures and structures that shape our field. It is not just about who is at the table, it is about how the table is built, who shapes the agenda, and how inclusive environments spark new ways of thinking. Advancing gender equality and equity is the spark that drives innovation and builds resilience. When diverse perspective and lived experiences converge, science becomes more adaptive, creative, and capable of meeting complex global challenges. By empowering every voice, we amplify the spirit of exploration that propels science forward. Drawing on global data, proven practices and Dr. Tsang's lived experiences, this presentation will highlight the leadership approaches, cultural shifts and acts of allyship that are redefining what progress in science looks like. The future of science depends on the bold choices we make today - to lead with equity, act with integrity, and build a scientific community where everyone can thrive. Join this session and be part of building that hopeful future together.

ADVANCING GENDER EQUALITY IN TAIWANESE CHEMISTRY COMMUNITY

Chao-Ping Hsu^{a,b*}

^aInstitute of Chemistry, Academia Sinica, Taipei, Taiwan 11529

^bVice President, The Society of Taiwan Women in Science and Technology

**Corresponding author: cherri@sinica.edu.tw*

Abstract

Despite the growth in chemistry research in Taiwan, women faculty representation is declining, especially in prestigious research institutions. In this presentation, I plan to highlight three initiatives addressing this trend: (1) Since 2021, the Society of Taiwan Women in Science and Technology (TWiST) has held the annual Women in Science & Technology (WiST) Convention for five consecutive years, uniting women from government, industry, and academia with National Science and Technology Council (NSTC) and presidential support; (2) Small gatherings of women chemists and physicists have evolved into an official NSTC two-day workshop on Career and Gender Equality since 2021, attracting nearly 100 attendees annually and providing thematic discussions and networking for gender minorities at all career stages; (3) A Mentor-Mentee program launched in 2023 with private donations to the Taiwan Chemical Society offers one-on-one support for junior chemists pursuing academic excellence. While women remain underrepresented in Taiwanese STEM fields, these evolving efforts represent an ongoing commitment to equality, diversity, and inclusion in the scientific community.

CHEMISTRY FOR GENDER EQUALITY IN AFRICA FOR ACHIEVING SUSTAINABLE DEVELOPMENT GOALS

Jane Catherine Ngila*

^aUniversity of Johannesburg, Department of Chemical Sciences

^bAfrican Foundation for Women & Youth in Education & STI

*Corresponding author: jcngila2015@gmail.com

Abstract

The African continent faces many challenges such as poverty and inequalities, education, health and unemployment challenges, climate change impact on food and nutrition security, digital infrastructure and connectivity gaps.¹ To address these problems towards achieving sustainable development goals (SDGs), Africa and indeed the world, need science, technology, and innovation (STI) as enablers for development and to foster economic growth. Chemistry is a central discipline that underpins the physical, material, and biological world, and it finds application across multiple fields, including health, food, water, energy, and other industrial processes, hence playing a significant role in addressing the SDGs.² Science fields such as chemistry are crucial to drive innovation, increase productivity, and enhance competitiveness, ultimately leading to a more prosperous and equitable society.³ By fostering a more inclusive environment in STI, the world can unlock the full potential of talent, leading to more creative solutions and greater innovation, ultimately boosting economic growth. Thus, gender gaps in science, technology, engineering and mathematics (STEM) fields must be addressed so as to include more women in science and in decision making fora. In Africa, societal and cultural biases, limited access to education and resources, and systemic issues, significantly hinder women's participation in STEM fields. Gender digital divide further hinders women from accessing affordable solutions and full participation in driving sustainable development.⁴ This paper discusses policy frameworks and case studies of African women in STEM and digital spaces, and how these impact the implementation of SDGs in the continent, and the role chemistry can play in finding solutions.

Keywords: gender equality, STEM in Africa, chemistry and SDGs, science technology and innovation

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ADVANCING GENDER EQUALITY IN CHEMISTRY: CHALLENGES, OPPORTUNITIES, AND FUTURE DIRECTIONS

Ghada Bassioni

*Saxony Egypt University for Applied Science and Technology;
on leave from Chemistry Division, Faculty of Engineering, Ain Shams University, Cairo, Egypt
Corresponding author: provost@seu.edu.eg; ghada_bassioni@eng.asu.edu.eg*

Abstract

As a female scientist and academic leader of a new university, I've witnessed the persistent challenges and biases that women face in STEM fields. Despite progress, gender disparities continue to affect women's participation, retention, and advancement in chemistry and related fields.¹ This highlights the need for inclusive environments, policies, and practices that promote gender equality in chemistry. Drawing from my experiences and research, the importance of addressing unconscious bias, stereotypes, and structural barriers that hinder women's success in chemistry becomes visible. Mentorship programs are instrumental to foster a culture of inclusivity and diversity. In the field of chemistry, proper education strategies encourage gender equality. Ensuring that chemistry curricula include diverse perspectives, examples, and case studies that showcase women's contributions to the field enhances female students' activity. The impact of workshops and seminars on topics such as leadership, communication, and negotiation skills, tailored to women in chemistry have been tremendous. Providing women students with research opportunities, internships, and projects that allow them to apply theoretical knowledge and develop practical skills have been instrumental.² The implementation of these strategies have shown how positive female students react. By promoting gender equality in chemistry, we have proven that the full potential of talented individuals can be unlocked, to drive innovation, and address global challenges. This abstract aims at showcasing ongoing efforts to advance gender equality in chemistry and related fields, ensuring a more diverse, equitable, and inclusive future.

Keywords: gender equality in chemistry; diversity; mentorship

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RESEARCH DIRECTIONS IN CURRENT AND FUTURE CHALLENGES IN LINE WITH SDG 6: CLEAN WATER AND SANITATION TOWARDS WATER SECTOR TRANSFORMATION 2040 (AIR 2040)

Mohd Zaki Mat Amin^a

^aNational Water Research Institute of Malaysia

*Corresponding author: zaki@nahrim.gov.my

Abstract

Malaysia's commitment to Sustainable Development Goal 6 (SDG 6) — ensuring the availability and sustainable management of water and sanitation for all — is closely aligned with the national Water Sector Transformation 2040 (WST 2040) agenda. In the face of escalating water demand, pollution, resource scarcity, and the growing impacts of climate change, the need for a forward-looking, research-driven approach has become increasingly critical. This paper identifies and critically evaluates both current and emerging research directions necessary to address the complex challenges related to clean water and sanitation in Malaysia within the WST 2040 framework. Key research themes include the strengthening of Integrated Water Resources Management (IWRM), the deployment of smart water technologies, utility digitalization, and the adoption of nature-based solutions to enhance ecological resilience. Particular attention is given to addressing rural-urban disparities in service access, socio-political dynamics in water governance, and the role of public-private-community partnerships. The integration of real-time data analytics, decentralized wastewater treatment systems, and circular water economy principles is also highlighted as fundamental to driving sustainable transformation. The study underscores the importance of cross-sectoral collaboration, coherent policy frameworks, and capacity building at both institutional and grassroots levels. Through interdisciplinary research and innovation, Malaysia has the potential to foster a more inclusive, resilient, and future-proof water sector. Aligning national research priorities with WST 2040 not only reinforces Malaysia's SDG 6 commitments but also positions the country as a regional leader in sustainable and equitable water management. This paper proposes a comprehensive and action-oriented research agenda to guide policymaking, academic discourse, and stakeholder engagement toward achieving universal access to clean water and sanitation by 2040.

Keywords: Sustainable Development Goal 6 (SDG 6), Water Sector Transformation 2040 (WST 2040)

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APPLICATION OF BIMETALLIC OXIDES FOR WATER/WASTE REMEDIATION

Bharat Kumar Allam^{a*}

^aDepartment of Chemistry, Faculty of Basic Sciences, Rajiv Gandhi University (A Central University), Rono Hills, Doimukh, Arunachal Pradesh, India

**Corresponding Author: allambharatkumar@gmail.com; bharat.allam@rgu.ac.in*

Abstract

The global scarcity of clean drinking water and the persistent accumulation of plastic waste pose serious environmental and public health concerns. Rapid industrialization, population growth, and climate change have exacerbated water contamination and plastic waste generation, necessitating the development of advanced and sustainable remediation strategies. Conventional water treatment and plastic waste management technologies often fall short of meeting the rising demand for safe water and effective pollutant removal, particularly given the increasingly stringent environmental regulations.

In response to these challenges, bimetallic oxides have emerged as highly efficient materials for water purification and plastic waste remediation. These materials leverage the unique properties of two distinct metal oxides, resulting in enhanced physicochemical characteristics, superior catalytic activity, and multifunctional capabilities. Their synergistic effects enable improved adsorption, redox reactions, and photocatalytic degradation of a wide spectrum of contaminants, including heavy metals, organic pollutants, and microbial pathogens. Furthermore, their structural tunability, cost-effectiveness, and adaptability to various environmental remediation processes make them highly promising candidates for sustainable applications.

This talk highlights recent advancements in bimetallic oxide-based materials, emphasizing their mechanisms of action and technological innovations in wastewater treatment and plastic waste remediation. It also examines key challenges related to scalability, environmental safety, and the feasibility of integrating these materials into large-scale treatment systems. By harnessing the unique properties of bimetallic oxides, we strive to develop more efficient, eco-friendly, and sustainable solutions for mitigating water pollution and plastic waste accumulation.^{1–5}

Keywords: Water pollution, plastic waste, bimetallic oxides, pollutant removal, cost-effectiveness.

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***IN-SITU* RAMAN SPECTROSCOPY STUDY OF WATER AT ELECTRODE/ SOLUTION INTERFACE**

Yao-Hui Wang^{a,*}, Jian-Feng Li^{a,*}

^aCollege of Materials, Xiamen University, Xiamen, 361005, Fujian, China

**Corresponding author: yaohuiwang@xmu.edu.cn, li@xmu.edu.cn*

Abstract

Water is vital to life, and its importance is self-evident as it plays an essential role in practically every scientific field, especially on the surface of materials. A clear understanding of the structure of water at the solid/liquid interface is necessary for understanding and developing fundamental concepts in the surface-science, catalysis, and energy-science communities. More importantly, water molecules directly participate in important electrocatalytic reactions, such as hydrogen evolution, oxygen evolution, carbon dioxide/oxygen/nitrogen reduction, etc. These reactions typically occur at the electrode/solution interface and are driven by an applied potential. However, interfacial water is notoriously difficult to probe, owing to its location between two condensed phases, let alone at surfaces with external bias potentials applied and where electrocatalytically induced reactions can occur. Therefore, the structure of interfacial water and its role in electrocatalytic reactions, especially on a model catalyst single-crystal surface, remains a long-standing puzzle in electrochemical community.

Surface-enhanced Raman spectroscopy (SERS) is a highly sensitive in-situ characterization technique for studying the water at the electrode/solution interface. Since noble metals (Ag, Au, Cu) have an extremely strong SERS effect, previous studies have mainly focused on the surface of rough polycrystalline noble metal electrodes. The SERS signals of interfacial water cannot be directly observed on the surface of transition metals with better catalytic performance or on the surface of atomically smooth model single-crystal electrodes. By using the shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS) technique, we have successfully obtained in-situ Raman spectral evidence of the structural and quantitative changes of interfacial water molecules on the surfaces of materials such as Pd single crystals and graphene. The results show that as the potential shifts negatively, the interfacial water molecules gradually transform from a disordered and chaotic structure into a structure with two hydrogen atoms facing downward. The structure of water molecules with two hydrogen atoms facing downward exhibits a high degree of interfacial order, and this ordered structure accelerates the charge transfer efficiency of the hydrogen evolution reaction (HER). Our results provide strong support for the understanding of the electrode/solution interface.

Keywords: Interfacial water, Raman, SHINERS, Electrochemistry

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ASSESSMENT OF CHROMIUM LEVELS, HEAVY METAL CONTAMINATION, AND ECOLOGICAL RISKS FROM TANNERY WASTE DISPOSAL IN KENYA AND SOUTH AFRICA

Richard O. Oruko^a and Joshua N. Edokpayi^b

^a*Department of Ecology and Resource Management, University of Venda, South Africa*

^b*Water and Environmental Management Research Group, Faculty of Science, Engineering and Agriculture, University of Venda, South Africa*

**Corresponding author: Joshua.Edokpayi@univen.ac.za*

Abstract

Sub-Saharan African countries have introduced environmental policies to manage industrial pollution, but enforcement remains inadequate, and pollution levels are poorly monitored due to limited resources¹. This study evaluated potentially toxic heavy metal (HM) contamination and physicochemical properties of effluents and dumpsite soils from two tanneries, one in Kenya (KT) and another in South Africa (ST), across different seasons. Pollution levels and ecological risks in dumpsite soils were assessed using indices such as the geoaccumulation index (Igeo), contamination factor (CF), pollution load index (PLI), and potential ecological risk index (PRI). Results revealed that mean concentrations of total dissolved solids, chemical oxygen demand, and heavy metals (Cr, Cu, Fe, Ni, Zn, Cd) in effluents from both tanneries exceeded discharge guideline limits. Specifically, mean Cr concentrations in effluents were 1.82 mg/L (ST) and 7.90 mg/L (KT), while Cr (VI) concentrations in dumpsite soils were 0.31 mg/kg (ST) and 0.4 mg/kg (KT). Fe concentrations in KT soils (2498 mg/kg) surpassed acceptable thresholds set by the World Health Organization (WHO) and Food and Agriculture Organization (FAO). Pollution indices highlighted significant contamination, with mean PLI values of 5.3 (KT) and 1.6 (ST), indicating higher pollution at KT. Igeo values of 18 (KT) and 2.4 (ST) further underscored chromium contamination. PRI values showed moderate ecological risk for KT (174.8) and low risk for ST (57.4). Plants sampled at both sites exhibited elevated chromium levels, reflecting the contamination's impact on local ecosystems². The study emphasizes the need for improved effluent management and advanced treatment technologies for tannery waste³. Strengthening monitoring systems and enforcing compliance with industrial discharge regulations are critical for mitigating pollution and ecological risks in Kenya, South Africa, and broader sub-Saharan Africa³.

Keywords: Chromium effluent, Cr (VI), Ecological risk, Integrated pollution indices, Tannery dumpsites.

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ECO-FRIENDLY BIOSORPTION OF HEAVY METALS AND ANIONS BY *PLEUROTUS ERYNGII*: A SUSTAINABLE SOLUTION FOR WATER DECONTAMINATION

Farah Amin^{a*}

^aNational Centre of Excellence in Analytical Chemistry, University of Sindh, Jamshoro - 76080, Pakistan

*Corresponding author: farahamin00@gmail.com

Abstract

Environmental pollution is becoming a serious and challenging problem all over the world because of high level of industrial development and growth¹. Various industries discharge toxic heavy metals and anions into the environment that considerably enhanced the humiliation of marine environment and significantly threatens the ecosystem². These unwanted chemicals cause severe health problems, when they exceed the tolerance limit in water³⁻⁵. For this reason, the removal of toxic pollutants is the greatest challenge. Biosorption method based on utilization of microorganisms has been given a significant attention due to efficient, rapid, easier, less expensive and environment friendly properties of biosorbent material for the removal of toxins from aqueous solution⁶⁻⁸.

Owing to the significance of biosorption technique, the projected work is based upon the biological preparation of environmental friendly fungal biomass *Pleurotus eryngii* (*P. eryngii*) and their exploitation for the removal of selected toxic metal ions (Pb, Cd, Hg) and anions (F⁻, NO³⁻) from aqueous system. Before and after sorption the biomass were characterized by FTIR, AFM, SEM and EDX techniques to verify surface functionality and morphology, whereas the surface chemistry charge studies (pH_{pzc}) were carried out to measure the approx. pH at which biosorbent behave as cationic, anionic and neutral species. After optimization of experimental variables (concentration, time, temperature), isotherm (Langmuir, Freundlich, Temkin, D-R models), kinetic (pseudo first, pseudo second, intra particle diffusion models) and thermodynamic (enthalpy, entropy, Gibbs free energy) parameters were calculated. The presence of interfering ions during biosorption and re-usability studies after appropriate desorption were carried out. Response Surface Methodology (RSM) was also employed in selected part of the studies to decrease the number of experiments, improved product yields and reduced treatment time and overall research cost. For the application of *P. eryngii* on real water samples; toxic pollutant (metals / anions) contaminated samples were collected from river, canal, lake and streams of Sindh, Pakistan. It was evaluated that under optimal conditions (at natural pH values) selected ions were removed effectively underneath the permissible limits of World Health Organization (WHO) drinking water standards^{9,10}.

Keywords: biosorption, heavy metals, anions, toxic pollutant, isotherm.

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DEVELOPMENT OF THIN FILM POLYAMIDE WITH MODIFIED GRAPHENE OXIDE DERIVED FROM PETROLEUM INDUSTRIAL WASTE SUPPORTED PVDF MEMBRANE FOR EFFICIENT WASTEWATER TREATMENT

Mauliady Satria^a, Abd. Rahman Marlan^a, and Tawfik A. Saleh^{a*}

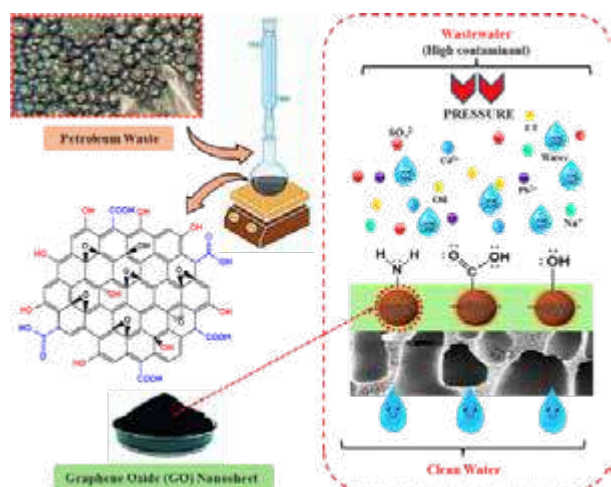
^aDepartment of Chemistry, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

Corresponding author: mauliadysatria@gmail.com

Abstract

Membrane-based separation methods are crucial for wastewater treatment, offering durability, efficiency, and stability. Reverse osmosis membranes with nanocomposites combine thermal, physical, and mechanical robustness with enhanced processability. Engineering membrane surface wettability is essential for separating complex oil/water mixtures and many contaminants such as heavy metals, dyes, and salts. In this study, petroleum waste-derived graphene oxide (GO) was used to minimize energy consumption and improve eco-friendliness. A hydrophobic polyvinylidene fluoride (PVDF) membrane was transformed into a superhydrophilic/underwater superoleophobic surface via spray coating method. A thin polyamide layer functionalized with triethylenetetramine-grafted GO (GO-TETA) was layered onto PVDF support to enhance its properties. The impact of incorporating 5% GO-TETA nanocomposites on the PVDF membrane's structure, morphology, antifouling, and superhydrophilicity was evaluated using a cross-flow permeation system. Advanced characterization techniques such as TEM, SEM/EDX, AFM, FTIR, XRD, and Raman spectroscopy validated structural, chemical, elemental, and morphological changes of the modified PVDF membrane before and after filtration test. For the results, the modified PVDF membrane exhibited excellent superoleophobicity (underwater oil contact angle (OCA) $\sim 145^\circ$) and superhydrophilicity (water contact angle (WCA) $\sim 0^\circ$). It demonstrated high permeate flux (~ 42 LMH), over 90% salt (NaCl and MgSO_4) rejection, over 93% heavy metal (Pb^{2+} , Cr^{3+} , Cd^{2+} , and Cu^{2+}) rejection, and over 97% hydrocarbon/organic solvent (pentane, isooctane, toluene, and hexadecane) rejection under high pressure (10 bar). The membrane maintained stability during an 8-hour cross-flow test, showcasing long-term use and antifouling properties. The GO-TETA nanocomposites enhanced superhydrophilicity, water permeability, surface roughness, and selective adsorption of heavy metals while blocking high containing salt solution. Ultimately, this study successfully converted petroleum waste into valuable GO nanosheet material for industrial wastewater treatment, offering a secure, eco-friendly, and cost-effective solution. It also advances sustainable practices by removing a broad range of environmental pollutants, contributing to a greener environment.

Keywords: PVDF membrane, graphene oxide, thin layer, wastewater, antifouling.



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EFFECT OF NATURALLY OCCURRING DOPING ACID TOWARDS POLYANILINE PROPERTIES AND CONTAMINANT REMOVAL

Michelle Li-Yen Lee^a, Ishak Ahmad^b, Sook-Wai Phang^{a*}

^aDepartment of Physical Science, Faculty of Applied Science,
Tunku Abdul Rahman University of Management and Technology (TAR UMT),
Jalan Genting Klang, Setapak, 53300 Kuala Lumpur, Malaysia.

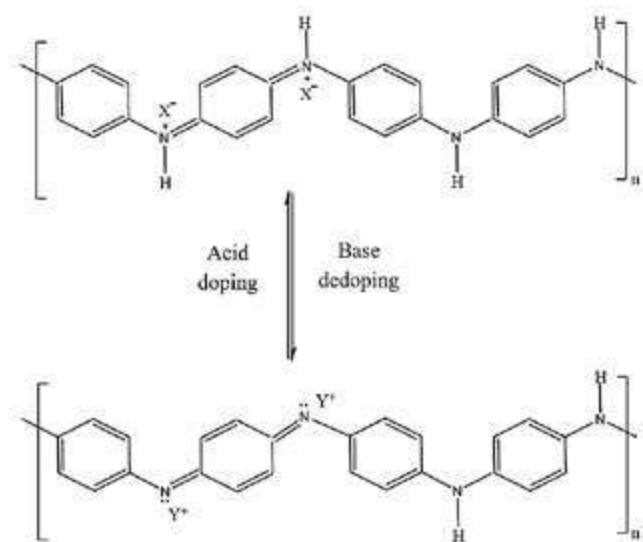
^bPolymer Research Centre (PORCE), Department of Chemical Sciences,
Faculty of Science and Technology, Universiti Kebangsaan Malaysia,
Bangi 43600, Selangor, Malaysia.

*Corresponding author: phangsw@taru.edu.my

Abstract

The tuneable and unique redox properties of polyaniline (PAni) make it a versatile candidate to be applied as contaminant adsorbent for wastewater treatment. In this research, naturally occurring doping acids namely acetic acid, benzoic acid, citric acid, formic acid, and tartaric acid are used to replace conventional use of hydrochloric acid for PAni doping. The chemical structure and oxidation state of differently-doped PAni samples were examined and confirmed by FTIR and UV-Vis analysis respectively. Different properties such as conductivity, morphology, surface area, and etc were observed for PAni doped with different acids. Furthermore, by altering the oxidation states of PAni, the cation and anion contaminant removal efficiencies of differently-doped PAni samples were measured. It is shown in this research that with the usage of different doping acids, PAni properties can be greatly tuned and modified due to different degree of PAni protonation. In addition, the morphological growth of PAni structure is also varied due to different steric effect and properties of dopant anion. These factors contributed to different cation and anion contaminant removal efficiencies measured for the different PAni samples.

Keywords: polyaniline, doping acid, cation removal, anion removal, polymer protonation



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ELECTRO-DRIVEN CYCLING FENTON CATALYSIS THROUGH THE ELECTRO-RESPONSIVE METAL-ORGANIC FRAMEWORKS FOR WATER PURIFICATION

Chao Yang^{a*}, Xiao-yan Li^{b,c}

^a School of Environmental Science and Engineering, Sun Yat-sen University, Guangzhou, China

^b Department of Civil Engineering, The University of Hong Kong, Pokfulam, Hong Kong, China

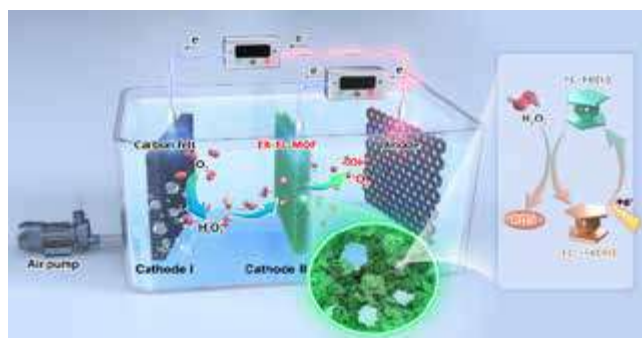
^c Institute of Environment and Ecology, Tsinghua Shenzhen International Graduate School, Tsinghua University, Shenzhen, China

*Corresponding author: yangch327@mail.sysu.edu.cn

Abstract

The electro-Fenton process is a promising technology for eliminating emerging organic pollutants from water. However, its potential is hindered by the lack of cathode materials with essential cycling catalytic functionality for sustained Fenton reactions. Here we present a 2D electro-responsive ferrocene-based MOF (ER-Fc-MOF) as an electro-driven cycling catalyst for the electro-Fenton process, effectively addressing the challenges of H_2O_2 activation and Fe(II) catalyst regeneration. The ER-Fc-MOF cathode on the Ni foam possessed electro-responsive property, and high stability for long-term operations (>150 h). Notably, for treating SMX in wastewater, the ER-Fc-MOF cathode-based electro-Fenton system exhibited a significantly high degradation rate constant (0.079 min^{-1}) at 1.5 V, which was 4.6 times that obtained without the DC supply and 3.7 times that of the non-responsive FeNi-MOF cathode-based system at 1.5 V^{-1} . More importantly, it enabled direct electron transfer for the cathodic reduction of Fc-Fe(III) to achieve continuous recycling of Fc⁺-Fe(III)/Fc-Fe(II) within the Fc sandwich structure, realizing a stable SMX degradation efficiency of 96.2% in long-term operation. The ER-Fc-MOF cathode generated both radical ($\bullet\text{OH}$) and non-radical ($^1\text{O}_2$) ROS, enabling effective organic oxidation over a wide pH range (3.0-9.2) in complex water matrices. The realization of electro-driven Fe(III)-Fe(II) cycling in the ER-Fc-MOF cathode enables the continuous activation of H_2O_2 without the consumption of the electrode and catalyst materials, which addresses the fundamental drawbacks of the conventional Fenton processes. The innovative use of electro-driven cycling catalysis will greatly improve the efficiency and sustainability of advanced oxidation for water pollution control. This research provides valuable insights into the development of electro-responsive MOF cathodes for the electro-Fenton process, paving the way for more effective and sustainable electrochemical technologies for water pollution control and alternative water resources.

Keywords: Cycling catalysis; electro-Fenton; electro-responsive metal-organic frameworks; emerging organic pollutants; wastewater treatment



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PROCESS OPTIMIZATION FOR THE REMOVAL OF LEAD (II) FROM AQUEOUS SOLUTION USING SPENT COFFEE GROUNDS VIA RESPONSE SURFACE METHODOLOGY

Mac Michael M. Rubio^{a*}

^a*Department of Physical Sciences, College of Science, University of the Philippines Baguio, Governor Pack Road, Baguio City, Benguet 2600, Philippines*

**Corresponding author: mmrubio1@up.edu.ph*

Abstract

Heavy metal contamination, particularly lead pollution, has become a global concern due to its environmental and health risks. This study evaluates the potential of spent coffee grounds (SCG) for lead (II) removal from aqueous solutions. Using response surface methodology (RSM) with a Box-Behnken design (BBD), key adsorption parameters—initial lead concentration, pH, and adsorbent dosage—were optimized. Complete lead (II) removal (100%) was achieved at 100 ppm, pH 5.54, and 10 g/L adsorbent dosage, with a 2.47% relative error validating the RSM model ($R^2=0.9701$). Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR) and Scanning Electron Microscopy coupled with Energy Dispersive X-ray Spectroscopy (SEM-EDS) analyses confirmed the adsorption of lead (II) onto the surface of the SCG after the adsorption process. The process was well described by the Langmuir isotherm model ($R^2=0.99928$) and followed pseudo-second-order kinetics ($R^2=0.99924$). The SCG adsorption capacity of 68.03 mg/g highlights its potential as an eco-friendly, low-cost, and sustainable adsorbent for lead (II) removal from aqueous solution.

Keywords: spent coffee grounds, lead (II), removal, adsorption, response surface methodology

ASSESSMENT OF VARIOUS PHOTOTHERMAL MATERIALS FOR SOLAR VAPORIZATION

^{1&2}Najma Memon* and Shakeela Abbas

¹National Centre of Excellence in Analytical Chemistry, University of Sindh, Jamshoro, Sindh-Pakistan.

²Faculty of Applied Sciences, UCSI University, KL, Malaysia

*Corresponding author: najma.memon@usindh.edu.pk

Abstract

Water scarcity is a serious challenge and causes problems for two billion people worldwide. Tapping into solar energy seems to be a viable and sustainable solution for the ongoing global challenges of water scarcity and clean energy shortage. However, low evaporation rates often compromise the natural mechanism of solar energy-driven water evaporation. Therefore, the current study presents use of an interfacial solar evaporator to achieve localized heating on the water vapor-liquid interface by photothermal materials. To develop an Efficient Interfacial Solar evaporator, two types of photothermal materials known as Plasmonic Janus Membrane imprinted with CuO nanoparticles and biochar were prepared and characterized with the help of SEM, BET, FT-IR and UV-visible spectroscopy. These photothermal materials show high activity, contain functional groups with aromatic rings and hydroxyl groups, have a porous structure and large surface area. Interfacial solar evaporator developed during experimental work which contains photothermal material floating on the surface of water and experimental work was done by utilizing normal sunlight. The mass change of water was calculated by using an Electronic Balance and a Thermometer was used to check temperature changes after each hour. It has been found that the temperature increase is highest in Plasmonic Janus Membrane imprinted with CuO nanoparticles than in biochars due to the Surface Plasmon Resonance Effect of CuO nanoparticles. The evaporation rate was compared in which biochar shows highest evaporation rate of 0.433 Kg/m²/h in comparison to CuO imprinted Plasmonic Janus Membrane with 0.347 Kg /m²/h while water without photothermal material shows 0.214 Kg/m²/h evaporation rate. It is concluded that the highest evaporation rate of biochar is due to its hierarchical porous structure and the presence of aromatic functional groups. Hence, biomass-derived interfacial solar evaporation provides a cost-effective solution to water scarcity.

Keywords: Nanoheaters; thermal radiation; water purification; low-density carbons

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ANALYTICAL, MODELLING AND NANOTECHNOLOGY TECHNIQUES FOR WATER QUALITY MANAGEMENT

Jane Catherine Ngila*

^aUniversity of Johannesburg, Department of Chemical Sciences

*Corresponding author: jengila2015@gmail.com

Abstract

Access to safe drinking water is a universal human right as per UN sustainable development goal #6.¹ In Sub-Saharan Africa (SSA), only 39% of the population has water connected to their homes and in the region's rural areas, this figure drops to just 19%.² The water challenges include, climate change, water pollution, poor water management, etc. We have used analytical techniques combined with nanotechnology for water quality monitoring. These include emerging technologies such as advanced oxidation processes (AOPs), ultra and nano filtration, adsorption/ biosorption, etc. Our research group has developed nanotechnology-based methods for water treatment and purification strategies to remove water pollutants using biomass and nanocomposite filters based on electrospun nanofibers and membranes.^{3,4} Our work achieved degradation of organic compounds through dechlorination and photodegradation of pesticide residues in water. We have enhanced detection limits and robustness of analytical techniques, multivariate-based optimization techniques.⁵ We have employed integrated approach to wastewater treatment plants (WWTPs)' design, using mathematical modelling and simulation techniques, resulting in a framework for plant modelling of activated sludge and biofilm, metabolic approaches, fate of micropollutants' removal processes and utilization of the sludge.⁶

Keywords: analytical techniques, mathematical modelling, nanocomposite membranes, advanced oxidation processes, water treatment

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REUSABLE CHEMICALLY FUNCTIONALIZED FLUORESCENT CRYOGELS: A SUSTAINABLE APPROACH TO ENVIRONMENTAL MONITORING

Zeynep Munteha Sahin^{a,b*}, Ilke Gurol^{a,b}

^aGebze Technical University, Department of Chemistry, Kocaeli 41400, Türkiye

^bTÜBİTAK Marmara Research Center, Materials Technologies, TUBITAK, Kocaeli, 41400, Turkey

*Corresponding author: zsahin@gtu.edu.tr

Abstract

Mercury pollution is a critical global issue, severely impacting ecosystems and human health. Once released into water bodies, mercury undergoes bacterial conversion into methylmercury, a highly toxic and bioaccumulative form. This contaminant accumulates in aquatic organisms and enters the food chain, posing significant health risks, particularly to children, where exposure can lead to neurological damage and developmental disorders. Effective and sustainable detection methods are essential to mitigate mercury contamination and protect water resources for future generations.^{1,2}

This study aimed to develop reusable fluorescent ion-sensing cryogels for the selective and rapid detection of Hg²⁺ in water. The cryogels were synthesized via post-functionalization with different comonomers and fluorescent molecules, and their composition was optimized to enhance detection performance. The effects of comonomer type and fluorescent molecule concentration on the limit of detection (LOD) and naked-eye detection sensitivity were investigated. Variations in hydrophilicity and reactivity of the comonomers influenced ion diffusion, while changes in fluorescent molecule concentration affected detection capability. Fluorescence-based detection enabled the identification of Hg²⁺ at levels as low as 2×10^{-8} g/mL, demonstrating high sensitivity. The synthesized cryogels were evaluated in aqueous solutions to assess their sensitivity and selectivity. Cryogels with a higher proportion of hydrophilic comonomers exhibited increased softness, leading to faster ion diffusion and improved detection efficiency. Additionally, the materials could be easily regenerated by simple washing with water, offering a sustainable approach for repeated use. The combination of selective recognition, rapid response, and straightforward regeneration demonstrated that these fluorescent cryogels could serve as an efficient tool for mercury detection in water.

Developing affordable, reusable, and water-based sensing materials contributes to a more sustainable approach for mercury monitoring, reducing environmental and economic burdens. The implementation of such materials can enhance large-scale water quality assessments, supporting global efforts to mitigate heavy metal contamination and protect public health.

Keywords: mercury detection, fluorescent molecules, ion sensing, detection in water, reusability

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DIAGNOSIS OF WATER RESOURCES IN THE CITY OF BANDUNDU IN THE DEMOCRATIC REPUBLIC OF CONGO

Valentin Tembe Mwela¹

Red Cross Higher Institute of Health Sciences of Bandundu

**Corresponding author: tembevalentin@gmail.com*

Abstract

The city of Bandundu with its 1.100.000 habitants, located at the confluence of the Kwango, Kwilu and Kasai rivers, has significant surface water reserves and ground water in quantity and quality, including the management, protection and value are dependent on new challenges imposed by sustainable development and climate change. This study aims to provide decision makers, researchers and donors with scientific information on the characteristics of waters of the Kasai, Kwango, and Kwilu rivers, to date, there is a lack of data base and in addition a lack of human resource to deal with the difficulties of managing water resource in the country. Thus, the characterization of the water resources of the Kasai, Kwango and Kwilu rivers is done using the isotopic tool and conventional hydrogeological techniques. The physico-chemical parameters (p^H , electrical conductivity, oxygen, temperature, major ions are measured.)

Kasai river

Date	Heure	ph	T ^{°c}	Conductivity us/cm	O ₂ Mg/l	NO ₃ Mg/l	NO ₂ Mg/l	PO ₄ mg/l	SO ₄ Mg/l	Alk Mg/l	CO ₂ Mg/l	Seechi cm
16/11/2018	9h00	10,025	29	28,3 us/cm	4,53 60,5%	4,5	0,021	0,31	1,6	7,5	16,5x2	40cm

Kwango river

Date	Heure	ph	T ^{°c}	Conductivity us/cm	O ₂ Mg/l	NO ₃ Mg/l	NO ₂ Mg/l	PO ₄ mg/l	SO ₄ Mg/l	Alk Mg/l	CO ₂ Mg/l	Seechi cm
16/11/2018	11h00	9,553	28,5	45us/cm	4,82 68,8%	8,1	0,071	0,5 4	7,1	12	15,5 x2	38cm

Kwilu river

Date	Heure	ph	T ^{°c}	Conductivity us/cm	O ₂ Mg/l	NO ₃ Mg/l	NO ₂ Mg/l	PO ₄ mg/l	SO ₄ Mg/l	Alk Mg/l	CO ₂ Mg/l	Seechi cm
16/11/2018	12h00	9,245	28,3	9,2us/cm	5,61 70,2%	0,6	0,032	0,37	1,8	3,0	12 x2	79cm

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SCALABLE INTERMITTENT COLD PLASMA-MICROBUBBLE TECHNOLOGY FOR DISINFECTION OF WASTEWATER IN MEAT PROCESSING

Xuehua Zhang^{a,*}, Deepak Panchal^a, Ziya Saedi^a, Qiuyun Lu^a,

^a Department of Chemical and Materials Engineering, University of Alberta, 9211 116 Street NW, Edmonton, Alberta T6G 1H9, Canada

*Corresponding author: Xuehua.zhang@ualberta.ca

Abstract

Cold plasma-bubble (CPB) technology, leveraging air and electricity, presents a sustainable solution for wastewater treatment, yet scalability remains a critical barrier. Here, we address this challenge by integrating portable, low-power cold plasma generators with engineered venturi tubes to enable spontaneous microbubble formation in a continuous flow system. This design achieves stable microbubble generation across variable flow rates, scaling treated water volumes to 120 L while maintaining energy efficiency comparable to small-scale applications. A universal linear correlation ($R^2 > 0.95$) between microbubble total surface area and activation efficiency—quantified via methyl orange degradation—was identified, providing a predictive framework for system optimization. The system demonstrated broad-spectrum disinfection, achieving >6 -log CFU/mL reduction of Gram-negative, Gram-positive, and antibiotic-resistant bacteria in both synthetic and real wastewater. For real-world validation, poultry processing wastewater underwent flotation-based pre-treatment, reducing turbidity (66%) and organic load (57%) to minimize interference, followed by intermittent microbubble-enhanced cold plasma activation (MB-CPA). Intermittent MB-CPA enhanced antibacterial efficacy 1.3-fold over continuous operation, enabling rapid inactivation (10–15 min) of high bacterial loads (~ 5.7 -log CFU/mL reduction in 3.5 L; ~ 5 -log in 10 L). Scalability was evidenced by a robust linear relationship ($R^2 = 0.96$) between treatment volume and exposure time, confirming predictable performance across scales. The integrated approach—combining pre-treatment with intermittent MB-CPA—successfully addressed the complex matrix of industrial wastewater, achieving compliance with stringent discharge standards. By bridging the gap between laboratory-scale CPB systems and industrial demands, this work establishes a transformative strategy for scalable, energy-efficient water treatment. The technology's adaptability to fluctuating flow rates, coupled with rapid disinfection and minimal energy penalties, positions it as a viable solution for meat processing and other industries requiring high-throughput, chemical-free wastewater remediation.

Keywords: Cold plasma; Microbubbles; Flow; Wastewater; Food Processing

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INDIUM OXIDE/GOLD/CARBON NANOCOMPOSITE FOR EFFICIENT VISIBLE LIGHT DRIVEN PHOTODEGRADATION OF DYES

Teck Hock Lim^{a*}, Pui Munn Wong^a, Richard D. Tilley^b, Joon Ching Juan^c

^a Department of Physical Science, Faculty of Applied Sciences,
Tunku Abdul Rahman University of Management and Technology

^bUniversity of New South Wales, Sydney, Australia

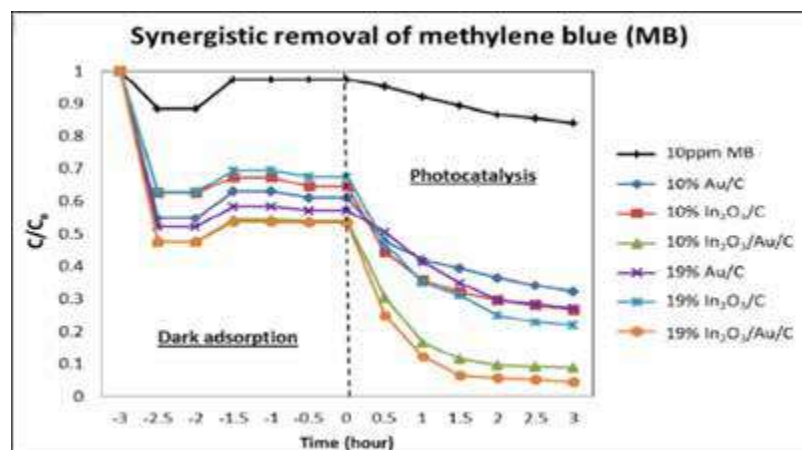
^cNANOCAT, Universiti Malaya

*Corresponding author: limth@tarc.edu.my

Abstract

As a pre-discharge treatment, solar-powered photocatalytic degradation of harmful dyes is gaining traction because it uses less chemicals and could be paired with direct sunlight or simulated solar radiation powered by green energy.¹ This requires designer photocatalysts that could absorb both the UV and visible range.² The work reported here focused on modifying sub-10 nm In nanoparticles (NPs)³ with AuCl₃ in a reducing environment to afford a homogenous In NPs/Au NPs mixture. The mixture was loaded on fiber glass and heated to 400 °C to produce In₂O₃/Au NPs which showed a strong absorption between 300-700 nm. The method was extended to carbon black to produce a new In₂O₃/Au/C nanocomposite with improved water dispersibility. The In₂O₃/Au/C nanocomposite was structurally characterized with a combination of PXRD, FESEM and HRTEM. TGA was employed to confirm the masses of In₂O₃/Au loaded on carbon which was controlled at 10% and 19%. Photocatalytic degradation performance of the nanocomposite was evaluated using methylene blue (MB) under simulated solar irradiation. The synergistic effect between In₂O₃ and Au NPs significantly enhanced the photocatalytic performance: A 10% In₂O₃/Au loaded on carbon led to a degradation efficiency > 90%. The photocatalytic degradation process was found to follow a 2nd-order kinetics and the incorporation of Au into In₂O₃ increased the photocatalytic-degradation rate-constant by more than 5 folds. The formation and degradation mechanisms would be discussed.

Keywords: Photocatalytic-degradation, In₂O₃/Au/C nanocomposite, Synergistic-effect, Methylene blue.



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THERMALLY AND CHEMICALLY STABLE ISOPOROUS BLOCK COPOLYMER MEMBRANES

Michael Appold^a, Sofia Rangou^a, Brigitte Lademann^a, Sarah Glass^a, Volkan Filiz^{a*},

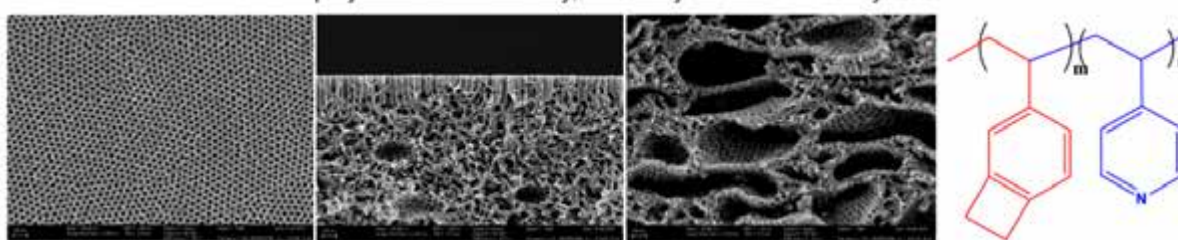
^a Helmholtz-Zentrum Hereon, Institute of Membrane Research, Max-Planck-Str.1, 21502 Geesthacht, Germany.

*Corresponding author: Volkan.filiz@hereon.de

Abstract

Amphiphilic block copolymers are promising candidates for the fabrication of ultrafiltration membranes with an isoporous integral asymmetric structure. The membranes are typically fabricated by the combination of block copolymer self-assembly and the non-solvent-induced phase separation (SNIPS) process resulting in isoporous integral asymmetric membranes. Certainly, all these membranes lack thermal and chemical stability limiting the usage of such materials. Within this study, the fabrication of completely cross-linked isoporous integral asymmetric block copolymer membranes is demonstrated by UV cross-linking resulting in chemical and thermal stable ultrafiltration membranes. The UV cross-linking process of PVBCB-*b*-P4VP (poly(4-vinylbenzocyclobutene)-*b*-poly(4vinylpyridine)) block copolymer membranes in dependency of irradiation time, intensity, distance between membrane and UV source and the wavelength is investigated. Furthermore, it is shown that the penetration depths can be increased by soaking the membranes in wave-guiding solutions before UV cross-linking is carried out.

Keywords: Anionic polymerization, block copolymers, isoporous membrane, ultrafiltration membrane, self-assembly



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WATER PURIFICATION FROM MICROTOXICANT DICLOFENAC BY CATALYTIC HYDRODECHLORINATION

Ekaterina Lokteva^{a,*}, Elena Golubina^a, Igor Kaplin^a

^a*Lomonosov Moscow State University, Moscow, Russia*

**Corresponding author: e.lokteva@rambler.ru*

Abstract

Chlorinated organic compounds pose a significant risk to the environment. Many pharmaceuticals, among them the non-steroidal anti-inflammatory drug diclofenac (DCF), contain chlorine atoms. With industrial wastes and metabolic products, DCF enters wastewater, groundwater, and then drinking water. It is persistent in the environment, and poorly amenable to treatment by activated sludge [1]. Catalytic hydrodechlorination (HDC) is an attractive method of removing DCF from industrial and hospital wastewater because the MAC of the reaction product, 2-anilinophenylacetate, is much higher than that of diclofenac, and the by-product, dilute HCl, is not hazardous [2]. This report describes the comparison of palladium catalysts on ordered mesoporous carriers (SBA-15 type) based on SiO₂ unmodified and modified by the ZrO₂. By methods of temperature-programmed reduction and XPS it is shown that palladium on such carriers which is able to be reduced by hydrogen from oxide under very mild conditions (30°C), effectively performs HDC of diclofenac in aqueous solution at 30°C, and very high TOF values are achieved for catalysts with very low palladium content. For example, for 0.1wt%Pd/ZrSBA after reduction at 30°C and at 300°C, the TOF (268 and 248 h⁻¹ correspondingly) has similar value, which is significantly higher than that of a disordered carrier catalyst of the same composition with a high palladium content (0.86%Pd/ZS, TOF = 0.04 h⁻¹), and than that of 0.1wt%Pd/SBA-15, which was not modified with zirconium dioxide. According to TEM, the size of palladium nanoparticles is higher in the 0.1wt%Pd/ZrSBA catalyst (10-80 nm vs. 5 nm in the 0.86%Pd/ZS). It is shown that the 0.1wt%Pd/ZrSBA catalyst works efficiently and stably in the flow regime.

Keywords: diclofenac, hydrodechlorination, palladium catalyst, SBA-15, zirconia

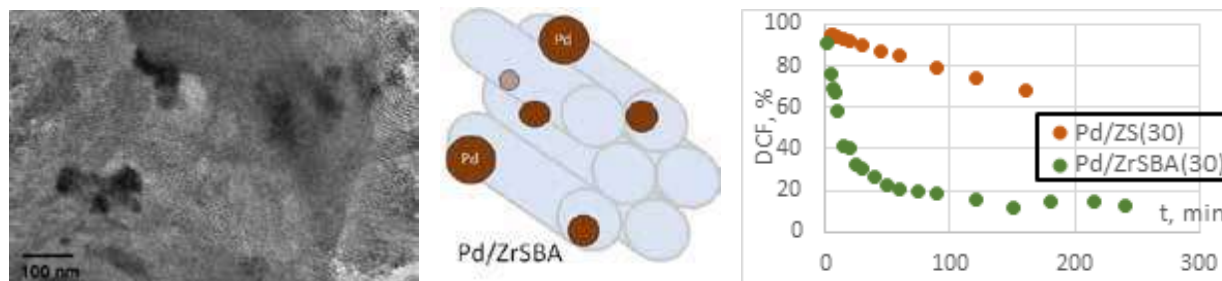


Fig. 1: TEM image and structure of Pd/ZrSBA, catalytic performance in HDC of DCF at 30°C (0.05 g of catalyst, reduced at 30°C with H₂, H₂ 0.6 L/h, 150 mg/L DCF in water, 15 mL).

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VISIBLE-LIGHT-DRIVEN DEGRADATION OF TETRACYCLINE USING $\text{CaFe}_2\text{O}_4/\text{CuWO}_4$ COMPOSITE: SYNTHESIS, CHARACTERIZATION, AND MECHANISTIC INSIGHT

Harsha S Rangappa^{a,b}, Chuxia Lin^{b*}, Subrahmanyam Challapalli^{c*}

^aCenter for Interdisciplinary Programs, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana, India-502285.

^bCentre for Regional and Rural Futures, Faculty of Science, Engineering and Built Environment, Deakin University, Burwood, VIC-3125, Australia.

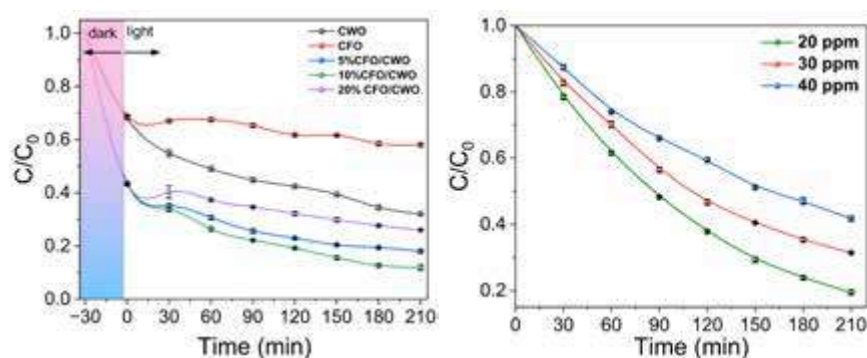
^cDepartment of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana, India-502285.

*Corresponding author: chu.lin@deakin.edu.au and csubbu@iith.ac.in

Abstract

The presence of emerging contaminants (EC) in aquatic environments has raised significant concerns because of their toxicity and resilience against traditional treatment approaches. A novel calcium ferrite (CaFe_2O_4) and copper tungstate (CuWO_4) composite photocatalyst was synthesized in this study using a two-step procedure that included hydrothermal treatment followed by sol-gel combustion. The physicochemical properties of the material were characterized using various techniques, such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), Brunauer Emmett Teller (BET) surface area analysis, Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). Tetracycline (TC), commonly found in EC, was chosen as the target pollutant for assessing photocatalytic performance. The findings indicated that the composite catalyst demonstrated significant superiority over its individual components, leading to enhanced pollutant degradation rates due to improved light absorption and effective charge carrier separation. The enhanced performance can be linked to the advantageous band alignment observed between CaFe_2O_4 and CuWO_4 , which promoted effective charge separation and transfer. Superoxide radicals, hydroxyl radicals, and electrons have been identified as significant radicals in the degradation mechanism. Furthermore, the composite demonstrated remarkable stability and reusability across numerous cycles, highlighting its potential for real-world application in wastewater treatment. These findings are crucial in the advancement of sustainable remediation of antibiotic-contaminated water through the development of photocatalysts that are powered by visible light and that are efficient.

Keywords: Water pollution, organic pollutants, sustainable treatment, catalysis, solar light driven.



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ECO-FRIENDLY ENZYME WASH ON DENIM GARMENTS AND ECONOMIC PROSPECTS

Waziha Farha^{a*}, Umme Habiba Rahman^b

^a*Department of Textile Engineering, Bangladesh University of Business and Technology (BUBT), Rupnagar, Mirpur-2, Dhaka, Bangladesh*

^b*Department of Economics, Bangladesh University of Business and Technology (BUBT), Rupnagar, Mirpur-2, Dhaka, Bangladesh*

^{*}*Corresponding author: dfarha@bubt.edu.bd, wazihafarha@gmail.com*

Abstract

Denim fabric is in high demand nowadays in the fashion industry among all ages. With the continuous development in the global fashion business, denim washing is progressively making its way onto the list of essential processes. Hence, promoting a sustainable, eco-friendly enzyme wash typically requires lower temperatures and shorter processing times, reducing water consumption (supporting SDG 06) and energy usage. Enzymes are biodegradable and harmless to the environment. Enzyme wash helps to soften the denim fabric, resulting in a comfortable and luxurious feel, promoting sustainable production (SDG 12). The research includes collecting enzymes, raw material, and chemicals and proceeds to de-sizing & neutralizing the fabric. Maintenance of the required temperature for different enzymes (Acid, Neutral, & Granular), followed by the extraction of the processed garments and transfer to the drying section, which ends with evaluating the quality denim garments through different textile testing quality methods. All the tests support enzyme wash, which is less harmful to the ecosystem and reduces the overall environmental impact of textile processing. This study compares the cost of using enzymes (a more eco-friendly alternative) versus traditional chemical treatment (Bleach wash & acid wash). Although enzymes are more expensive upfront, they may reduce overall costs in the long run. Moreover, eco-friendly enzyme wash benefits the environment as well as offers economic opportunities through sustainable innovation in the textile industry contributing to SDG 12.

Keywords: Denim, acid wash, enzymes, enzyme wash, sustainability, SDG, eco-friendly.

ENHANCING THE ADSORPTION OF CADMIUM FROM AQUEOUS SOLUTIONS USING TITANIUM DIOXIDE-DOPED CARBON NANO ADSORBENTS VIA RESPONSE SURFACE METHODOLOGY

Hamza A. Asmaly^{a,*}, Nassereldeen Kabbashi^a, Ma'an Fahmi Al-Khatib^a, Md Zahangir Alam^a

^a Chemical Engineering and Sustainability, IIUM Gombak, 53100 Kuala Lumpur

*Corresponding author: hamza2t@gmail.com

Abstract

A novel carbon-based nanocomposite incorporating carbon nanotubes, nanofibers, and titanium dioxide (Titania) was developed for the efficient removal of cadmium from aqueous solutions. The synthesis employed an impregnation technique optimized through central composite design to enhance adsorption performance. Comprehensive characterization confirmed the successful modification of the adsorbent. Scanning Electron Microscopy (SEM) revealed improved morphology and surface structure, while Energy Dispersive X-ray (EDX) analysis verified and quantified Titania loading. Fourier Transform Infrared Spectroscopy (FTIR) confirmed the presence of Titania-associated functional groups within the carbon matrix. Surface area analysis using the Brunauer-Emmett-Teller (BET) method showed a significant increase from 92 m²/g in pure carbon nano adsorbents (CNA) to 139 m²/g after Titania loading, and further to 184 m²/g after optimization. Thermal Gravimetric Analysis (TGA) demonstrated good thermal stability of the modified composite. The initial cadmium adsorption capacity was 34.29 mg/g at a concentration of 50 ppm using 20 mg of the adsorbent. Process optimization improved this capacity to 52.0 mg/g at 100 ppm with 50 mg dosage. Further refinement using Response Surface Methodology (RSM) predicted a capacity of approximately 53.0 mg/g under optimized conditions (130 ppm, 49 mg dosage), with experimental validation yielding 48.64 mg/g—an error margin of just 8.2%. Adsorption equilibrium data best fit the Langmuir isotherm model, indicating monolayer adsorption, while the kinetics were accurately described by the Pseudo First Order model. These findings demonstrate the effectiveness of the Titania-modified carbon nanocomposite as a high-performance, thermally stable adsorbent for cadmium removal from wastewater, highlighting its potential for sustainable water purification applications.

Keywords: Cadmium, Titanium oxide, Adoption and Carbon Nano Adsorbent.

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SEWAGE WATER SAMPLES ANALYSIS AS A TOOL FOR MONITORING ILLEGAL DRUGS

Nurfaizah Abu Tahrim*, Norfaizan Padli, Nor Hafizah Hashim

Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600

UKM Bangi, Selangor, Malaysia.

**Corresponding author: nfaizah@ukm.edu.my*

Abstract

Monitoring illegal drug use remains a complex challenge for public health and law enforcement agencies. This study explores the potential of sewage water analysis as a reliable and non-intrusive method for identifying drug consumption patterns within a population. The primary objective is to pinpoint geographic hotspots of drug use and quantify the concentration of specific illicit substances present in sewage samples. Sewage samples were collected from various locations across targeted urban zones. The samples were screened and analysed using liquid chromatography-timsTOF. The concentrations of commonly abused drugs were determined and compared across sampling sites. These data were then mapped to highlight areas with higher levels of drug residue, providing a spatial overview of consumption trends. This approach offers a real-time, community-level assessment of drug use, with potential applications in public health monitoring, policy-making, and resource allocation for harm reduction. The study reinforces the value of wastewater-based epidemiology as a complementary tool in addressing drug-related challenges.

Keywords: Sewage water, illegal drugs, wastewater-based epidemiology

DESIGN OF MESOPOROUS IODINE-DOPED G-C₃N₄ WITH CARBON VACANCIES FOR EFFICIENT VISIBLE-LIGHT-DRIVEN TETRACYCLINE REMOVAL

Bao Lee Phoon^a, Wai Kit Tang^c, Chin Wei Lai^a, Chia-Yun Chen^{b,c}, Supakorn Boonyuen^d, Joon Ching Juan^{a,*}

^a Nanotechnology & Catalysis Research Center (NANOCAT), IPS Building, Institute for Advanced Studies (IAS), Universiti Malaya, 50603 Kuala Lumpur, Malaysia.

^b Department of Materials Science and Engineering, National Cheng Kung University, Tainan 70101, Taiwan

^c Hierarchical Green-Energy Materials (Hi-GEM) Research Center, National Cheng Kung University, Tainan 70101, Taiwan.

^d Department of Chemistry, Faculty of Science and Technology, Thammasat University, Pathumthani, 12120, Thailand

^e Department of Chemistry, Faculty of Science, Universiti Malaya, Kuala Lumpur 50603, Malaysia

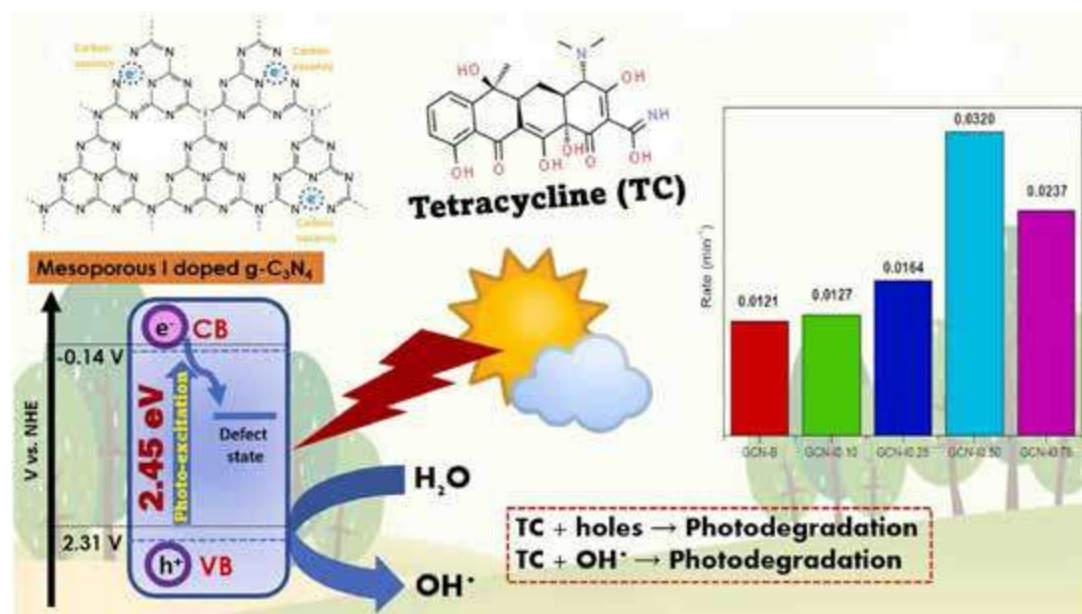
*Corresponding email: jcjuan@um.edu.my

Abstract

Antibiotics are widely used to treat bacterial infections in humans. However, residues of these compounds have been increasingly detected in the environment [1], posing serious ecological and health risks. The human body only metabolizes 25–70% of administered antibiotics, while the rest are excreted through sweat, urine, and feces [2]. Among various antibiotics, tetracycline (TC) is commonly used due to its affordability and effectiveness. It is employed not only in human medicine but also in veterinary applications and as a growth promoter in poultry farming. Unfortunately, TC is environmentally persistent and difficult to remove [3]. Its residues have been found in lakes, ponds, rivers, and hospital effluents, with river water showing concentrations as high as 255×10^2 ng/L [4]. Such contamination has been linked to health issues like impaired bone and tooth development in children [5] and hepatotoxicity in pregnant women [6]. The ineffectiveness of conventional wastewater treatment in eliminating TC highlights the need for better remediation approaches. Graphitic carbon nitride (GCN) has emerged as a promising photocatalyst for antibiotic degradation in wastewater. However, its photocatalytic efficiency is hindered by rapid electron–hole recombination, low surface area, and limited visible light absorption. In this study, mesoporous iodine-doped GCN (GCN-I) with varying iodine content was synthesized. The optimal sample, GCN-I0.50, achieved 99.8% TC degradation within 150 minutes under visible light ($\lambda > 420$ nm), a 2.64-fold improvement over pristine GCN. This enhancement is attributed to the introduction of iodine and carbon vacancies, which improve charge separation and reconstruction of the GCN framework. The mesoporous structure and increased surface area (63.76 m²/g) also enhance TC adsorption and degradation. Additionally, the structural distortion and smaller band gap (2.45 eV) promote n– π^* transitions, enabling effective photocatalysis under visible light. GCN-I0.50 demonstrates both high efficiency and stability for TC removal.

Keywords: Iodine, graphitic carbon nitride, photocatalyst, tetracycline, mesoporous

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INVESTIGATION AND COMPARISON OF PLANT MEMBRANE FILTRATION FOR WATER PURIFICATION

Diyana Kamarudin^{a,b*}, N. Awanis Hashim^c, Nurfaizah Abu Tahrim^{a,b}

^a *Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia.*

^b *Pusat Penyelidikan dan Analisis Air (ALIR), Fakulti Sains dan Teknologi, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.*

^c *Department of Chemical Engineering, Faculty of Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.*

^d *Center for Separation Science and Technology (CSST), Faculty of Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.*

*Corresponding author: diyana.k@ukm.edu.my

Abstract

This study investigates the effectiveness, sustainability, and relative performance of plant-based membrane filtering systems for water treatment, particularly in relation to traditional polymeric membranes. The study examines natural membranes obtained from cassava stems, investigating their viability as economical, biodegradable options for water purification. The xylem tissue of the cassava plant was examined for its capacity to eliminate diverse pollutants, such as synthetic colours and microbiological contaminants. Experimental assessments were performed to evaluate essential aspects like filtration efficiency, flow rate, pore size distribution, and structural durability under various operating situations. The findings indicate that cassava xylem displays efficient filtration capabilities, especially in decreasing turbidity and microbial contamination, while sustaining an adequate flow rate for small-scale uses. Its biodegradable characteristics and extensive availability augment its appropriateness for use in resource-constrained environments or emergencies when traditional filtration technologies may be unattainable. Cassava-based filters present a favourable equilibrium between efficacy and ecological sustainability when contrasted with manufactured membranes. This work provides significant insights into the advancement of biomimetic, plant-derived water treatment technologies and advocates for more investigation into plant-based materials as feasible alternatives for decentralised and sustainable water purification systems.

Keywords: cassava plant, E coli, water quality, Xylem tissue, polymeric filtration

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AFFORDABLE CLEAN WATER USING ADVANCED MATERIALS

Thalappil Pradeep

Indian Institute of Technology Madras, Chennai 600 036

**Corresponding author: pradeep@iitm.ac.in*

Abstract

Sustainable nanotechnology is important for providing contaminant-free water to humanity. I will present the discovery of affordable and sustainable nanomaterials to selectively scavenge arsenate and arsenite ions (and others) in water to bring their concentrations below the drinking water limits and its development into a technology. The solution, popularly called AMRIT (meaning elixir in Sanskrit), is now delivering 80 million litres of arsenic-, iron- and uranium-free water every day, conforming to international standards to 1.3 million people at the cost of 2.1 paise (US\$0.00026) per litre, lowest in the world. This technology has been approved for national implementation. We have developed several other technologies for sensing contaminants and their removal. A glimpse into these activities and directions for future will be presented. Diverse aspects of the science of water in the form of droplets and ice are also fascinating and couple of them will be mentioned briefly.

Keywords: Clean water and sanitation, Drinking water, Nanotechnology, Nanomaterials, Sustainable chemistry



One among the 1700 community water purification units deployed in India using AMRIT technology.

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WATERLESS TEXTILE DYEING: A SUSTAINABLE SOLUTION FOR A WATER-SCARCE FUTURE

Md. Ibrahim

Bangladesh University of Business and Technology (BUBT)

Corresponding author: ibrahimmahmud9740@gmail.com

Abstract

The persistent reliance on substantial water and chemical usage in conventional textile dyeing processes presents a stark contrast to the growing global awareness of water scarcity and environmental sustainability. This paper explores the emergence of innovative waterless dyeing technologies as a promising paradigm shift. We examine the principles and potential of supercritical carbon dioxide (scCO₂) dyeing, a method that utilizes pressurized and heated CO₂ as a solvent to directly infuse dyes into textiles, eliminating the need for water and significantly reducing chemical waste. Furthermore, we discuss alternative air dyeing techniques that offer another avenue for water-free coloration with potential energy savings. While current limitations such as material compatibility (primarily polyester) and initial equipment costs exist, the broader implications of widespread adoption of these technologies are profound. The transition to waterless dyeing holds the potential to drastically conserve water resources, minimize pollution, and contribute to a more sustainable and environmentally conscious textile industry, aligning with increasing consumer demand for eco-friendly apparel. This analysis highlights the transformative potential of these advancements, suggesting a future where traditional, water-intensive dyeing methods may become obsolete, much like the evolution from basic mobile phones to sophisticated smartphones.

Keywords: Waterless Dyeing, Supercritical CO₂, Air Dyeing, Sustainable Textiles, Environmental Impact.

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POLYHYDROXYALKANOATE-BIOCHAR BIOCARRIER: OPTIMIZING COMPOSITE FOR ENHANCED BIOFILM ATTACHMENT AND DEVELOPMENT

Phaik Ching Ang^a, Kumar Sudesh^b, Si Ling Ng^{a,*}

^aSchool of Chemical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia.

^bSchool of Biological Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia.

*Corresponding author: slng@usm.my

Abstract

Polyhydroxyalkanoates (PHAs), are promising environmentally friendly alternatives to conventional materials for biofilm carriers in enhanced wastewater treatment processes, owing to their biodegradability and biocompatibility. Recent studies have demonstrated their successful application biocarriers in moving bed biofilm reactors treating azo dye¹⁻³. The positive surface charge of PHA biocarrier aided in biofilm formation, and the stability of biofilm was supported by a high polysaccharide-to-protein ratio in the extracellular polymeric substances (EPS)¹. Biofilm growth was found to be improved by the incorporation of activated carbon into PHA². Azo dye decolorization was promoted, primarily due to the highly bioactive attached activated sludge and the anoxic zone within the biofilm that facilitated azo bond cleavage^{2,3}. Key microbial strains with bio-decolorization ability were identified¹. Building on these foundational successes, the current study aims to further improve PHA bioarrier for enhanced biofilm attachment and development by incorporating PHA with biochar derived from oil palm trunk waste, exploring various PHA compositions, PHA-biochar ratios. This approach seeks to optimize the biocarrier's properties and foster robust biofilm formation, contributing to efficient and sustainable biological wastewater treatment while also valorising agricultural waste resources.

Keywords: Polyhydroxyalkanoates; Biochar; Biofilm Carrier; Moving Bed Biofilm Reactor; Oil Palm Waste.



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ASSESSMENT OF SURFACE WATER QUALITY ASSOCIATED WITH UPSTREAM ARTISANAL MINING ACTIVITIES IN PREK TE AREA, CAMBODIA

Vibol Sao^{1*}, Chan Oeurn Chey², Socheata Korng², Davy Thoeun³, Kyoung-Woong Kim³

¹*Department of Environmental Engineering, Royal University of Phnom Penh, Federation of Russia Blvd, Tuol Kork, Phnom Penh, Cambodia*

²*Graduate School of Sciences, Royal University of Phnom Penh, Federation of Russia Blvd, Tuol Kork, Phnom Penh, Cambodia*

³*School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju 61005, Republic of Korea*

**Corresponding authors: Email: socheatakorng7@gmail.com*

Abstract

Mining activities may have significant impacts on water quality due to the release of various contaminants into the water sources. The objectives of this research are to examine the concentration of heavy metals and other elements in the water of Prek Te area in two seasons and to assess the human health risk of residents through drinking water pathway. Surface water sampling was conducted twice from March 5–11, 2023 (for the dry season) and from October 20–26, 2023 (for the rainy season). A total of 21 surface water samples were collected from different locations along the Prek Te area. The pH, Electrical Conductivity (EC), Dissolved Oxygen (DO) and Total Dissolved Solids (TDS) were measured on-site and the concentrations of Arsenic (As), Chromium (Cr), Nickel (Ni), Copper (Cu), Zinc (Zn), Cadmium (Cd) and Lead (Pb) were analyzed at the lab by Inductive Couple Plasma – Mass Spectrometry (Agilent, 8990). Analytical results showed that most of all parameters were ranked and lower than the guidelines of the World Health Organization (WHO) as well as Cambodia's drinking water quality standards (CDWQS) except As. Highest As concentration was 58.1 µg/L, followed by 22.0 µg/L and 10.8 µg/L in rainy season. For the health risk assessment, the hazard quotient (HQ) and Hazard Index (HI) were calculated to be higher than 1 for the children. Lifetime cancer risk (LCR) for children was found to be $> 1.8 \times 10^{-1}$ at a higher risk, followed by women of $> 1.2 \times 10^{-1}$ and men of $> 1 \times 10^{-1}$ for As. It may be concluded that children are more susceptible than adults to the health risks as a result of intaking contaminated water. Therefore, a monitoring program and appropriate drinking water treatment to remove contaminant such as As may be urgent to ensure a safe drinking for residents living along the Prek Te area.

Keywords: Artisanal mining, Heavy metal, Health risk, Prek Te area, Cambodia.

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ENSURING DATA INTEGRITY IN VOLATILE ORGANIC COMPOUND (VOC) ANALYSIS: A QUALITIES ASSURANCE APPROACH FOR RIVER WATER ASSESSMENT

Jamilah, K. *, Nasehir Khan, E.M.Y., Hazwani J, Mohd Fauzan A. T

National Water Research Institutes of Malaysia (NAHRIM), 43300 Seri Kembangan, Selangor, Malaysia.

** Corresponding author: jamilahkarim@nahrim.gov.my*

Abstract

Volatile Organic Compounds (VOCs) are a significant group of pollutants in river systems, often originating from industrial discharges, agricultural runoff, and urban wastewater. This study focuses on quality assurance (QA) measures in the monitoring and assessment of VOC contamination in Malaysian river water. Accurate identification and quantification of VOCs are critical due to their toxicity, persistence, and potential to harm aquatic ecosystems and human health. The study emphasizes the implementation of strict QA protocols, including standardized sampling, sample preservation, and analytical procedures using Gas Chromatography-Mass Spectrometry (GC-MS). Quality control steps such as field blanks, duplicates, and instrument calibration ensure data integrity and reproducibility. The findings highlight the importance of reliable monitoring systems in supporting environmental decision-making and regulatory compliance. This poster outlines the QA framework used in VOC studies and provides recommendations for improving data reliability and environmental protection strategies in Malaysia's riverine environments.

Keywords: Volatile Organic Compounds; quality assurance; Accurate identification; analytical procedures; regulatory compliance

PYROLYSIS: AN INNOVATIVE ALTERNATIVE FOR ALUM SLUDGE TREATMENT

**Nur Izzati Md Saleh^{a*}, Muhd Shahril Nizam Ismail^a, Muhammad Abdullah^a,
Nasehir Khan E.M Yahya^a**

^aNational Water Research Institute of Malaysia

*Corresponding author: nurizzati@nahrim.gov.my

Abstract

Human health relies heavily on hygiene particularly clean water, to prevent water disease. Water treatment plants (WTP) play a crucial role as it requires process like coagulation-flocculation, sedimentation, filtration, and disinfection to remove contaminants. Aluminum-based coagulants are commonly used during the process and it produces significant alum sludge which classified as scheduled waste in Malaysia. Traditional disposal methods like landfilling require substantial space and pose environmental risks due to potential pollutant leaching. Hence, pyrolysis offers a promising solution for pollutant removal and heavy metal immobilization. This study investigated pyrolysis at 700°C for treating alum sludge and analyzed using proximate, Carbon Hydrogen Nitrogen and Sulphur (CHNS), Energy Dispersive X-Ray (EDX) and Scanning Electron Microscopy (SEM) analysis. CHNS analysis showed an increase in carbon content (from 0.42% to 1.33%) and a decrease in hydrogen, nitrogen, and sulphur after treatment, indicating the removal of volatile organic components. Proximate analysis supported these findings, revealing a reduction in volatile matter (from 9.32% to 6.87%) and an increase in ash content (from 88.61% to 91.73%) in the treated alum sludge. SEM images illustrated a significant change in morphology after pyrolysis, with the treated alum sludge exhibiting a more fragmented and porous structure compared to the smoother, aggregated surface of the raw sludge. This altered morphology observed in the SEM images correlates with the EDX results, which showed a significant reduction in aluminum content from 9.32% in raw sludge to 4.00% in treated alum sludge, indicating that the structural changes likely facilitate the decrease in aluminum content. In conclusion, pyrolysis can be an innovative and environmentally alternative for alum sludge treatment.

Keywords: pyrolysis, alum sludge, water treatment plant, scheduled waste, aluminum coagulant.

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PRETREATMENT OF WASTEWATER AND SLUDGE FOR ENHANCED METHANE PRODUCTION DURING ANAEROBIC DIGESTION

Mohamed Hasnain Isa

*Universiti Teknologi Brunei, Tungku Highway, Gadong, BE1410, Brunei Darussalam.
mohamed.isa@utb.edu.bn*

Abstract

Anaerobic digestion (AD) is a widely used biological process for the treatment of wastewater and sludge. It offers the benefit of renewable energy generation in the form of biogas, with methane as its primary component. The efficiency of methane production in AD is often limited by the slow hydrolysis of complex organic compounds, low biodegradability of certain organic substrates, and presence of compounds that inhibit microbial activity. These limitations reduce the overall biogas yield and impact the economic viability of the process, especially in the treatment of waste with high solids content. Various physico-chemical pretreatment methods can be employed to suitably alter the characteristics of the wastes prior to their anaerobic treatment. The pretreatment methods improve substrate solubilisation, enhance microbial accessibility, and increase wastes biodegradability, providing a favourable environment for methanogenic archaea. Practical considerations such as energy input, chemical usage, environmental impact, and cost-effectiveness must be made to ensure beneficial treatment of wastewater and sludge.

DEMONSTRATING SOLAR ETHYLENE PRODUCTION, REACTOR INTEGRATION IN MULTI-STEP CONVERSION FROM H₂O AND CO₂

Pau Farràs Costa^{a,*}

^a*School of Biological and Chemical Sciences, University of Galway, H91 CF50, Galway, Ireland.*

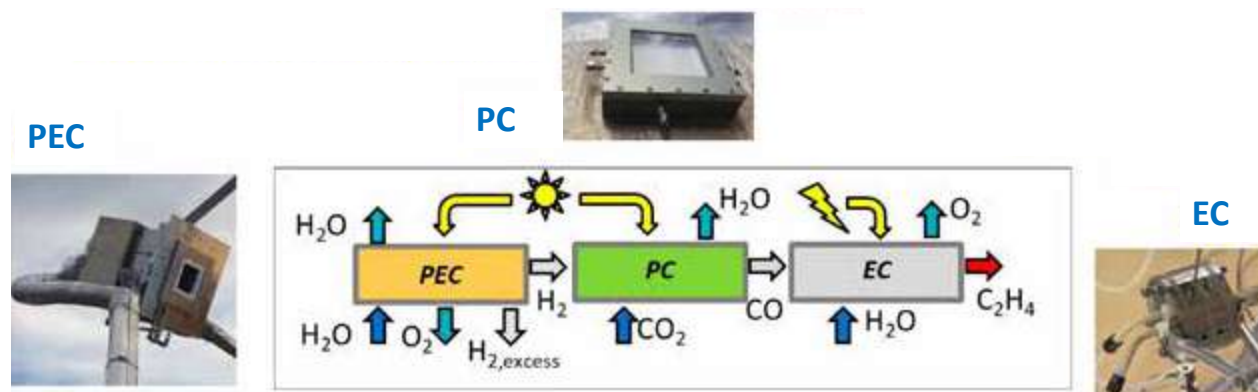
^{*}*Corresponding author: pau.farras@universityofgalway.ie*

Abstract

As part of the FlowPhotoChem project, the team of researchers have focused on model, design, construct and demonstrate a modular, integrated system of flow reactors (FPC system) for the production of useful chemicals using concentrated solar light with negative CO₂ emissions and minimal operational costs. Solar ethylene was selected as the product target of the demonstration because of its market value (\$1.30/kg) and the decarbonization potential on the current manufacturing process, steam cracking of ethane, which produces at least 1.5 kg CO₂/kg ethylene. In addition, we align with the Sustainable Development Goals (SDGs), in particular SDG 7.

In this presentation, the main results obtained in the project will be showcased, with special emphasis on the reactor development and scale-up, and the integration (for the first time), of three types of flow reactors. The photoelectrochemical (PEC) reactor was shown to produce solar hydrogen at a stable production rate of > 29 mol h⁻¹.¹ In the photochemical (PC) step, CO₂ hydrogenation to CO was accomplished using a Ru/STO (strontium titanate) photocatalyst with a production rate of 2 mol h⁻¹ g⁻¹ at 27% conversion yield.² Using a CO₂ trap, any unreacted CO₂ was captured so only CO entered the last, the electrochemical (EC) reactor. Powered by renewable electricity, CO was converted into ethylene using a 3-cell stack with a faradaic efficiency to the target product at 44% and a production rate,³ in the final fully integrated FPC system, of 0.06 mol h⁻¹, representing one of the highest reported rates for solar ethylene.

Keywords: photoelectrocatalysis, photocatalysis, electrocatalysis, modelling, materials



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Ce-Zr/Al-MCM-41 AS CATALYST FOR BIODIESEL PRODUCTION FROM DATE SEED OIL

Anita Ramli^{a,b,*}, Zainab Jibril^a, Khairulazhar Jumbri^a, Normawati Mohamad Yunus^a

^aFundamental and Applied Sciences Department, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia

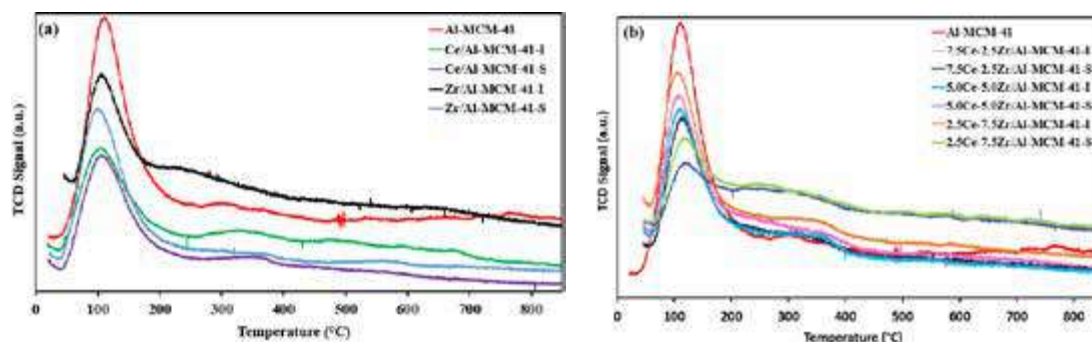
^bHICOE Centre for Biofuel and Biochemical Research Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak, Malaysia

*Corresponding author: anita_ramli@utp.edu.my

Abstract

Ce-Zr/Al-MCM-41 monometallic and bimetallic catalysts were prepared by impregnation and sonication-assisted methods for biodiesel production from Phoenix dactylifera L. seed oil. The physicochemical properties of the catalysts were studied using N₂ adsorption-desorption isotherms, X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), NH₃-TPD, and CO₂-TPD (Temperature Programmed Desorption). Results show that the ratio of CeO₂ and ZrO₂ loading has a significant influence on the catalytic performance of the Ce-Zr/Al-MCM-41 catalyst. Furthermore, sonication-assisted method improves the dispersion of CeO₂ and ZrO₂ particles. Response surface methodology based on the central composite design (RSM-CCD) was used for the optimization of biodiesel yield. The results show a good model fitting with an R² value of ~0.92%, from the analysis of variance. The optimum conditions were reaction temperature of 60.5 °C, reaction time of 3.8 h, catalyst loading of 4 wt.%, and methanol to oil molar ratio of 6.2:1 mol/mol for 93.83% biodiesel yield. Kinetics was studied at a reaction temperature range of 55 – 60 °C and reaction time 1 – 4 h. Pseudo-first order was the best-fitted model with activation energy (E_a) of 57.51 KJmol⁻¹ and the pre-exponential factor (A) of 1.00x10⁹ min⁻¹. Thermodynamic studies show positive Gibbs free energy of activation (ΔG[‡]) and enthalpy of activation (ΔH[‡]), and a negative entropy of activation (ΔS[‡]). The catalyst was reusable for 5 cycles with no significant difference in the FAME yield. The quality of FAME produced conforms to the ASTM D6751 and EN14214 standards.

Keywords: bimetallic catalyst; central composite design; Phoenix dactylifera L. seed oil; transesterification reaction



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OPTIMIZING 3D FUNCTIONALIZED GRAPHENE FOR SUPERCAPACITOR ELECTRODE

Kwok Feng Chong^{1,2*}, Soon Poh Lee³, Gomaa A. M. Ali⁴, Ellie Teo Yi Lih⁵

¹*Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang Al-Sultan Abdullah, Gambang, 26300 Kuantan, Malaysia*

²*Center for Advanced Intelligent Materials, Universiti Malaysia Pahang Al-Sultan Abdullah, 26300 Kuantan, Pahang, Malaysia*

³*Lee Kong Chian Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, Kajang, 43000, Selangor, Malaysia*

⁴*College of Marine Science and Aquatic Biology, University of Khorfakkan, Sharjah, United Arab Emirates*

⁵*Department of Science & Technology, Faculty of Humanities, Management and Science, Putra University Malaysia, Bintulu, Sarawak, Malaysia*

**Corresponding author: ckfeng@umpsa.edu.my*

Abstract

This study focuses on optimizing the structural and electrochemical properties of three-dimensional (3D) graphene xerogels for energy storage applications in supercapacitor electrodes. Reduced graphene oxide (rGO) xerogels were synthesized using L-ascorbic acid as a green reducing agent, eliminating the need for toxic hydrazine. The precursor graphene oxide (GO) sheets of varying lateral sizes were subjected to an ambient pressure drying technique, resulting in xerogels whose properties were strongly influenced by the GO sheet size. Smaller sheet sizes exhibited higher oxygen functionalities, which impacted the stacking behavior during xerogel formation. The optimized sheet size facilitated parallel sheet stacking, imparting mechanical strength capable of resisting capillary forces while retaining a high surface area and pore volume. These morphological characteristics contributed significantly to the superior electrochemical performance of the rGO xerogels. The work was further extended by introducing a light-responsive molecule, phenothiazine (PTZ), to form PTZ-functionalized rGO xerogels. Under UV irradiation, PTZ acted as a photo-reductant, transferring electrons to GO and simultaneously undergoing oxidation and covalent functionalization onto the rGO sheets. The optimal incorporation of PTZ resulted in a marked improvement in electrochemically active surface area and enhanced ion diffusion behavior, with diffusion efficiency increasing by up to 42%. The synergistic effect of pseudocapacitance from PTZ and the well-developed porous structure of the rGO xerogel underscores its potential as a high-performance supercapacitor electrode material.

Keywords: Graphene; Supercapacitor; Pseudocapacitance; UV light.

IN-SITU STUDY OF NANOCATALYTIC REACTIONS USING SURFACE-ENHANCED RAMAN SPECTROSCOPY

Hua Zhang*

College of Materials, Xiamen University, Xiamen, 361005, China

*Corresponding author: zhanghua@xmu.edu.cn

Abstract

Developing in-situ characterization methods with high-sensitivity and temporal-spatial resolution is of great significance for the deep understanding of catalytic reaction mechanisms and the rational design of efficient catalysts. Raman spectroscopy can provide rich structural information, especially for species located in the low-frequency region of the spectrum, thus is one of the most commonly used techniques in heterogeneous catalysis. However, its sensitivity is too low to achieve in-situ monitoring of the catalytic reaction process and trace surface intermediate species. To address this bottleneck, we have developed a highly sensitive SHINERS-satellite strategy by assembling nanocatalysts on the surface of nanoparticles with Au cores and oxide shells. In the SHINERS-satellite strategy, the Raman signals of surface species of the nanocatalyst (or even single-atom catalysts) can be greatly amplified, thus realizing in-situ Raman studies of the catalytic process and reaction intermediates. Using this strategy, we successfully achieved in-situ Raman characterization of species such as oxygen species in the catalytic oxidation process and revealed the influence of the catalyst's interfacial structure on oxygen activation. In addition, to address the low spatial resolution of conventional Raman spectroscopy, we developed a nanogap-enhanced Raman strategy, which enabled the in-situ characterization of hydrogen spillover at the nanometer scale. The results show that the spillover distance of active hydrogen species on the TiO_2 surface is about 50 nm, and hydrogen spillover is carried out by the formation and breaking of surface O-H bonds. Similar strategies have also been further extended to in-situ studies of photocatalysis and electrocatalysis.

Keywords: surface-enhanced Raman spectroscopy; in-situ study; nanocatalysis; intermediates; reaction mechanism.

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SUSTAINABLE ENERGY SOLUTIONS: OPTIMIZING BIODIESEL PRODUCTION THROUGH HETEROGENEOUS CATALYSIS USING ZnO/SiO_2 FROM AGRICULTURAL WASTE

Abd Rahman Marlan^{a,*}, Mohammad Nahid Siddiqui^b, Tawfik A. Saleh^c, Suriati Eka Putri^d,

^aDepartment of Chemistry, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia.

^bDepartment of Chemistry and IRC-Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia.

^cDepartment of Chemistry and IRC-Advanced Materials, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

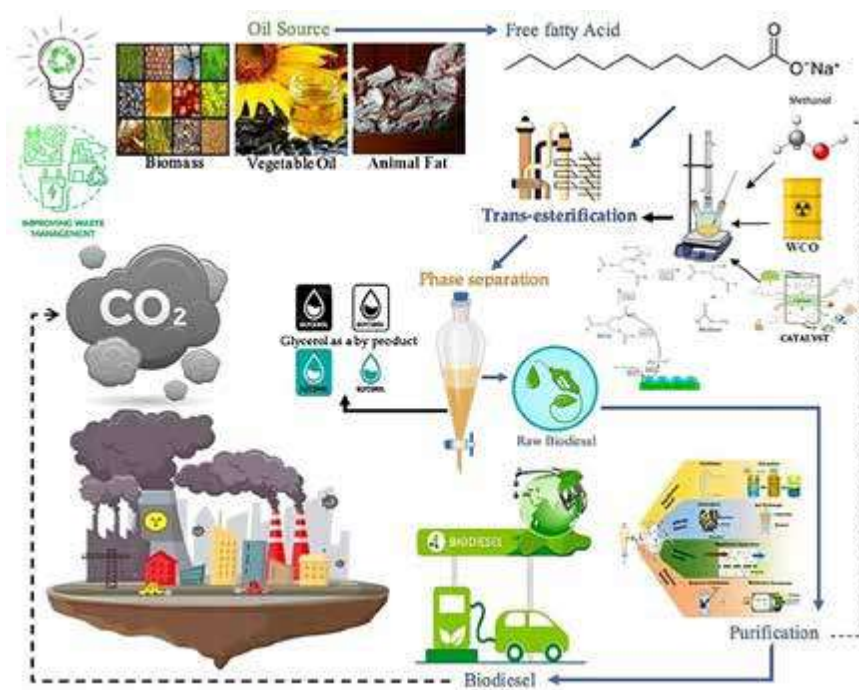
^dDepartment of Chemistry, Faculty of Mathematics and Natural Science, State University of Makassar, Makassar, Indonesia

*Corresponding author: g202206440@kfupm.edu.sa

Abstract

The escalating global energy demand, predominantly satisfied by fossil fuels, has led to severe environmental repercussions, including the emission of harmful pollutants and the depletion of non-renewable resources. This study explores the synthesis of green heterogeneous ZnO/SiO_2 derived from date leaves ash (DLA) as an innovative catalyst for biodiesel production, specifically using waste cooking oil (WCO) as feedstock. WCO, a prevalent byproduct in the food industry, poses significant environmental challenges, yet it offers a valuable opportunity for sustainable energy generation. The transesterification process in this study highlights additional techniques to improve the product by focusing on the intermediate species, which is essential to enhance the conversion of triglycerides in WCO to biodiesel, on the other hand enhanced by the application of the synthesized catalyst, which exhibits superior catalytic activity and stability. The research also highlights the advantages of using heterogeneous catalysts over traditional homogeneous catalysts, including ease of separation, reusability, and reduced environmental impact. The findings demonstrate that the DLA-derived ZnO/SiO_2 catalyst not only improves biodiesel yield but also contributes to waste management by repurposing WCO, thereby mitigating its adverse effects on public health and the environment. This work underscores the potential of green chemistry in developing efficient, eco-friendly catalysts that can significantly advance the biodiesel industry. This research advocates the integration of sustainable practices in energy production, emphasizing the importance of renewable resources in addressing the pressing challenges of energy sustainability and environmental protection. Ultimately, several highlights of this research have led to over 95% of WCO being converted to biodiesel using ZnO/SiO_2 -30 at 60 °C.

Keywords: green catalysis, DLA-derived catalyst, sustainable energy



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SYNERGISM, PYROLYSIS PERFORMANCE, PRODUCT DISTRIBUTION AND CHARACTERISTICS IN THE CO-PYROLYSIS OF DATE PALM WASTE AND POLYETHYLENE FOAM: HARNESSING THE POTENTIAL OF PLASTICS AND BIOMASS VALORIZATION

Ahmad Nawaz^a & Shaikh Abdur Razzak^{a,b}

^a *Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia*

^b *Department of Chemical Engineering, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia*

E-mail: ahmad.nawaz@kfupm.edu.sa

Abstract

The current methods of disposing of plastic waste, such as dumping or burning, create significant ecological problems and cause irreparable damage to valuable resources. This is especially true for plastics with complex structures, like polyethylene foams (PEF). This work focuses on how the plastic composition impacts the interactions, kinetics, and thermodynamic aspects during the co-pyrolysis of date palm waste (DPW) and PEF. Co-pyrolysis experiments were conducted at three different heating rates (10, 20, and 30 °C/min) and with varying ratios of biomass to plastic. The kinetic parameters were evaluated using different isoconversional techniques (Kissinger Akahira Sunose, Vyazovkin, and Ozawa Flynn Wall). The average value of activation energy based on the Vyazovkin model are 96.31, 216.33, 232.85, 382.69 and 206.47 kJ/mol for DPW, PEF, 75PEF25DPW, 25PEF75DPW, and 50PEF50DPW, respectively. The thermodynamic results showed that average difference between activation energy and enthalpy is 4.89, 6.02, 5.81, 5.36, and 5.61 kJ/mol for the DPW, PEF, 75PEF25DPW, 25PEF75DPW, and 50PEF50DPW, respectively. It is lowest for the DPW and highest for the PEF, whereas it is significantly lower for the mixes, indicating that the mixes consume less energy. The Criado's master plot suggested that co-pyrolysis of DPW and PEF followed D1 (one-dimensional) and D3 (three dimensional) reaction mechanism. Further, co-pyrolysis results from the fixed bed reactor confirmed maximum bio-oil yield (38.85 wt. %) was achieved at 50PEF50DPW ratio. The results of this study suggest that combining waste date palm with PEF could be a promising option for improving the co-pyrolysis process.

Keywords: Co-pyrolysis; Foam; Date palm; Kinetics; Thermodynamics; Sustainable development

DUAL-ISOLATION EFFECT OF BISMUTH IN NON-NOBLE BiNi ALLOYS FOR ENHANCED PERFORMANCE IN H₂O₂ ELECTROSYNTHESIS

Xiaomei Liu^a, Wenchao Peng^{a*}

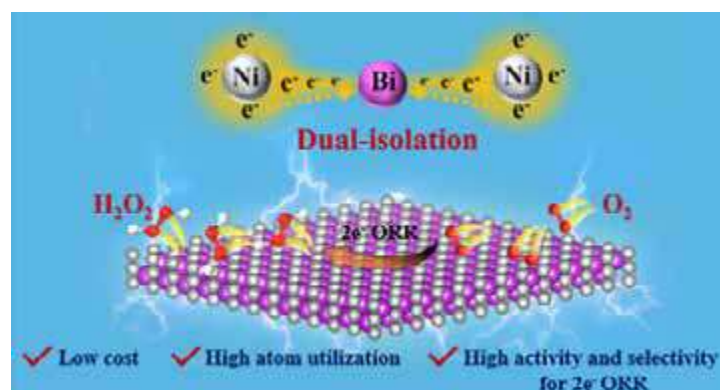
^a*School of Chemical Engineering and Technology, Tianjin University, China*

**Corresponding author: wenchao.peng@tju.edu.cn*

Abstract

Noble-metal alloys are high-efficiency 2e⁻ ORR catalysts for electrochemical production of H₂O₂.¹⁻³ However, the development of noble-metal alloys for H₂O₂ production is still in a bottleneck period due to their high cost, toxicity, low atom utilization, and limited reactivity.¹⁻³ To solve these dilemmas of noble-metal alloys, developing non-noble alloys can be an alternative. Herein, non-noble BiNi alloys with a uniform diameter of ~11 nm supported on carbon nanosheets (BiNi/C) is synthesized by a hydrothermal-pyrolysis method. The BiNi/C material exhibits high 2e⁻ ORR performance with an onset potential of 0.76 V vs RHE and a selectivity of ~98% in 0.1 M KOH. The H-cell tests deliver a high H₂O₂ yield of ~17 mM within 2 h at 0.4 V vs RHE. The synthesized H₂O₂ is then used in a fixed-bed Fenton process, the degradation efficiencies of RhB and BPA maintain at 100% and ~95% within 10 h, respectively. Theoretical calculations reveal that Bi can regulate the electronic structure of Ni in BiNi alloys through the “dual-isolation” effect of physical and electronic isolation. The adsorption energy for *OOH is thus decreased and side-on adsorption of *OOH on Ni sites is achieved. Furthermore, Bi atom itself with the lowest overpotential can also serve as high active site for H₂O₂ generation due to the dual-isolation effect. Our work provides a guidance for the synthesis of non-noble alloy catalysts for 2e⁻ ORR with high activity and selectivity.

Keywords: two-electron ORR, alloy catalysts, dual-isolation effect, high atom utilization, Fenton process.



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ECO-INNOVATIVE LDPE PHOTODEGRADATION VIA BiOCl-ZrO_2 NANOCOMPOSITES

Bharat Kumar Allam^{a,*}, Sushmita Banerjee^b, Samreen Sajad^b

^a*Department of Chemistry, Faculty of Basic Sciences, Rajiv Gandhi University (A Central University), Rono Hills, Doimukh, Arunachal Pradesh, India.*

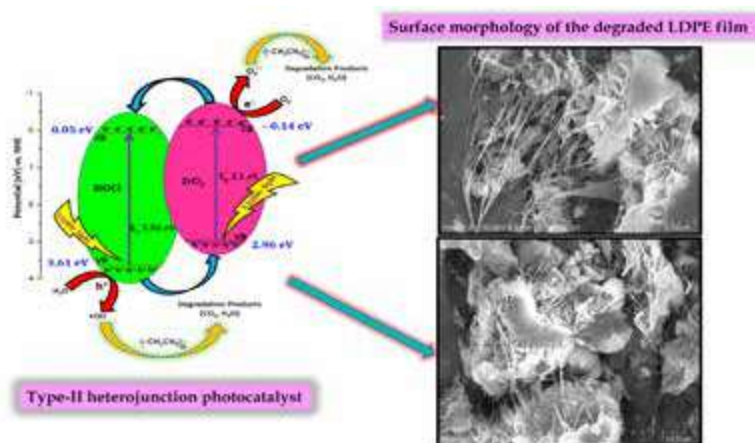
^b*Department of Environmental Sciences, School of Basic Sciences and Research, Sharda University, Greater Noida, Uttar Pradesh, India.*

*Corresponding author: allambharatkumar@gmail.com; bharat.allam@rgu.ac.in

Abstract

This study addresses plastic pollution by decomposing low-density polyethylene (LDPE) using a BiOCl-ZrO_2 nanocomposite under visible-light irradiation at room temperature. This sustainable approach aligns with Sustainable Development Goal 7 (SDG 7) by leveraging visible light, a clean energy source, for plastic waste reduction.¹ LDPE films were prepared via solution casting with BiOCl and BiOCl-ZrO_2 nanocomposites and subjected to visible-light irradiation for 24 days. Characterization techniques, including XRD, FT-IR, XPS, FE-SEM, TGA, BET, and UV-Vis DRS, confirmed the structural and functional properties of the nanocomposites. FT-IR analysis indicated a significant increase in the carbonyl index, revealing successful photodegradation of LDPE when combined with BiOCl-ZrO_2 . FE-SEM images showed substantial morphological changes, including perforations, highlighting LDPE decomposition on the nanocomposite surface. The weight reduction of LDPE@BiOCl-ZrO_2 (10 wt%) composite films reached 48.67% after 24 days, with the degradation rate influenced by nanocomposite concentration. The photodegradation mechanism relied on a type-II heterojunction photocatalytic system. The low bandgap of ZrO_2 (3.1 eV) facilitated electron transfer to BiOCl , while BiOCl 's large bandgap (3.56 eV) promoted hole transfer to ZrO_2 . This efficient charge separation reduced recombination, enhancing degradation performance. The process resulted in biodegradable LDPE fragments, contributing to reduced plastic pollution. The environmental impact was evaluated through carbon footprint estimation. Remediating 100 kg of plastic waste using this method generates an estimated 0.133 tons carbon footprint, highlighting its eco-friendly potential. This innovative approach demonstrates a scalable, energy-efficient, and sustainable pathway for mitigating plastic pollution, promoting the adoption of green nanotechnology for environmental remediation.

Keywords: BiOCl-ZrO_2 , photodegradation, plastic waste, Low-density polyethylene, carbon footprint.



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ENHANCED ELECTROCHEMICAL PERFORMANCE OF AQUEOUS ZINC-ION BATTERIES WITH POROUS BASIL-DERIVED CARBON AND NANOSTRUCTURED MnO_2 COMPOSITE CATHODES

Yuda Prima Hardianto ^a, Abdulmajid A Mirghni ^b, Syed Shaheen Shah ^c, Haneen Mohammed Alhassan ^b, Md. Abdul Aziz ^{b*}, Zain Hassan Yamani ^a

^a Physics Department, King Fahd University of Petroleum & Minerals, KFUPM Box 5047, Dhahran 31261, Saudi Arabia

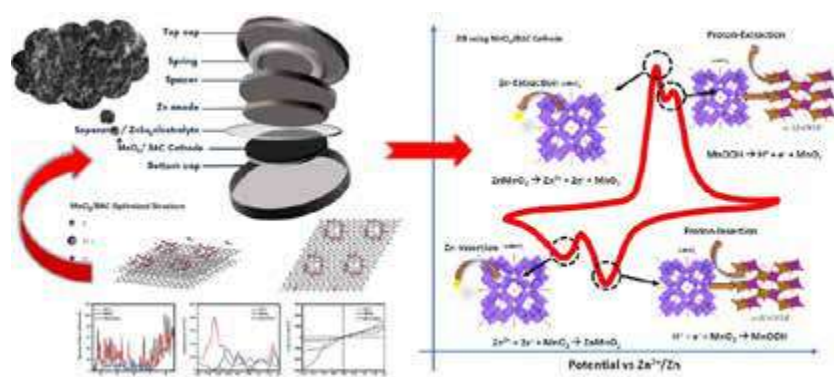
^b Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

^c Socio-Environmental Energy Science Department, Graduate School of Energy Science, Kyoto University, Yoshida Honmachi, Sakyo-ku, Kyoto 606-8501, Japan

*Corresponding author: maziz@kfupm.edu.sa

Abstract

This study introduces a novel composite cathode for aqueous zinc-ion batteries (ZIBs), leveraging porous basil-derived activated carbon (BAC) and nanostructured manganese dioxide (MnO_2) synthesized through a one-step hydrothermal process. For the first time, biomass-derived carbon is integrated with MnO_2 , resulting in enhanced electrochemical performance. The MnO_2 /BAC composite delivers a remarkable specific capacity of 237 mAh/g at 0.5 A/g, along with an energy density of 314 Wh/kg and a power density of 0.66 kW/kg, outperforming cathodes made from pristine MnO_2 or BAC. These improvements stem from reduced particle size and a synergistic balance of capacitive and diffusive charge storage mechanisms. Density functional theory calculations corroborate the experimental results, revealing the composite's superior quantum capacity (158.7 $\mu\text{C}/\text{cm}^2$) and quantum capacitance (80.4 $\mu\text{F}/\text{cm}^2$). Stability assessments highlight excellent cycle life, with >90% capacity retention and 100% Coulombic efficiency over 300 cycles. The exceptional performance is attributed to the material's unique nanostructure, high surface area (1090 m^2/g), and optimized porosity. This work establishes a new benchmark for sustainable and cost-effective cathode materials, significantly advancing ZIB technology for high-efficiency energy storage applications.



Keywords: Energy storage, Zinc-ion batteries, Porous carbon, Nanostructured MnO_2 , Composite materials

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ENHANCED HYDROGEN PRODUCTION USING CO, CU, AND NI-DOPED TiO₂ PHOTOANODE IN PHOTOELECTROCHEMICAL CELLS

Hayyiratul Fatimah Mohd Zaid^{a,b,*}, Nur Ain Atiqah Mohd Amin^{a,b}, Rashid Abdullayev^a

^aDepartment of Chemical Engineering, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak Darul Ridzuan, Malaysia

^bCentre of Innovative Nanostructures & Nanodevices (COINN), Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak Darul Ridzuan, Malaysia.

*Corresponding author: hayyiratul.mzaid@utp.edu.my

Abstract

Hydrogen production through photoelectrochemical (PEC) cells offers a sustainable energy solution by utilizing sunlight to split water into hydrogen, providing a clean alternative to fossil fuels with minimal energy loss. PEC cells integrate semiconductor materials with electrochemical systems to absorb light and generate the necessary electrical potential for water splitting. Titanium dioxide (TiO₂) is widely used in PEC applications due to its strong photocatalytic activity, chemical stability, and abundance. However, its wide bandgap (~3.2 eV) limits its absorption to only about 5% of sunlight, restricting its efficiency. To address this limitation, researchers explore doping TiO₂ with transition metals, integrating it with narrower bandgap semiconductors, and modifying surface structures to improve light absorption and charge separation. Doping metals such as cobalt (Co), nickel (Ni), and copper (Cu) into TiO₂ enhances its photocatalytic and electrocatalytic properties by optimizing its structural and electronic properties, thus improving hydrogen evolution efficiency. This study evaluates the effect of Co²⁺, Cu²⁺, and Ni²⁺ (2% wt.) doping on TiO₂ photocatalysts synthesized via the wet-impregnation method, with characterization performed using X-ray diffraction (XRD) to determine crystallinity and phase composition, field emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM) to analyze surface morphology and particle size, diffuse reflectance UV-visible spectroscopy (DR-UV-Vis) to assess optical absorption properties, Fourier-transform infrared spectroscopy (FTIR) to identify functional groups and chemical bonding, and X-ray photoelectron spectroscopy (XPS) to investigate surface chemical composition and oxidation states. The findings demonstrate that metal doping enhances light absorption, charge separation, and electrocatalytic activity, positioning doped TiO₂ as a promising material for PEC hydrogen production.

Keywords: Titanium dioxide; metal-doped; photocatalyst; photoelectrochemical cell; hydrogen production.

TARGETING BARRIERS IN ALKALINE WATER ELECTROLYSIS: CATALYSTS AND BINDER INNOVATIONS

Anzel Falch^{a*}, Adam Shnier^a, Tarisai Velepini^a, Fariya Moosa^a, Alex le Roux^a, Rueben Pfukwa^b and Jan J. Weigand^{b,c}

^aMolecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, 2001, South Africa, ^bDepartment of Chemistry and Polymer Science, Stellenbosch University, 7602, Stellenbosch, South Africa.

^cFaculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062, Dresden, Germany.

*Corresponding author: anzel.falch@wits.ac.za

Abstract

Electrocatalysis is essential for clean energy conversion, enabling technologies like fuel cells, rechargeable metal-air batteries, and electrolyzers. Extensive research has been focused on discovering high-performance electrocatalysts, leading to the development of new techniques to explore the structural and electrochemical properties of materials, as well as innovative strategies to enhance their performance. This presentation provides an overview of the field of electrocatalysis, with a particular focus on findings related to alkaline water electrolysis.

Water electrolysis is a promising method for producing green hydrogen. However, currently, only 2% of global hydrogen production is achieved through water electrolysis.¹ Alkaline Water Electrolysis (AWE) faces challenges due to slow reaction kinetics at both the anode and cathode². At the cathode, where hydrogen evolution occurs, performance is hindered by the slow initial water-dissociation step (Volmer). At the anode, the primary issue is the sluggish four-electron transfer process associated with the oxygen evolution reaction (OER).

To address these challenges, our research has focused on developing alternative catalyst compositions, structures, and exploring new binder systems. Mn-Ni oxide catalysts were synthesized for the OER using a low-temperature hydrothermal method at various Mn molar ratios, with disk inserts as electrode substrates. Linear sweep voltammetry (LSV) showed an overpotential of 330 mV (RHE) at 10 mA cm⁻² for the Mn-Ni (1:5) sample, demonstrating better performance than individual catalyst elements, indicating favorable synergy between these metals.

Currently, NafionTM is used as an ionomer in AWE despite its limitations in alkaline conditions, environmental toxicity, and high cost. We propose novel poly(vinyl alcohol) (PVA)-based binder systems to address these issues. Our results suggest that PVA enhances performance by improving the sluggish Volmer step in the alkaline hydrogen evolution reaction (HER), with initial findings indicating that PVA achieves competitive performance compared to NafionTM, offering a more affordable and environmentally friendly alternative.

Keywords: water electrolysis electrocatalysis, hydrogen, binder

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IMPACT OF IRON LOADING ON Ce-MODIFIED ALUMINA FOR BLUE HYDROGEN VIA CHEMICAL LOOPING

Achmad Ferdiansyah Pradana Putra^{1*}, Mohammad M. Hossain^{1,2,3}

¹Department of Chemical Engineering, ²Interdisciplinary Research Center for Refining and Advanced Chemicals,

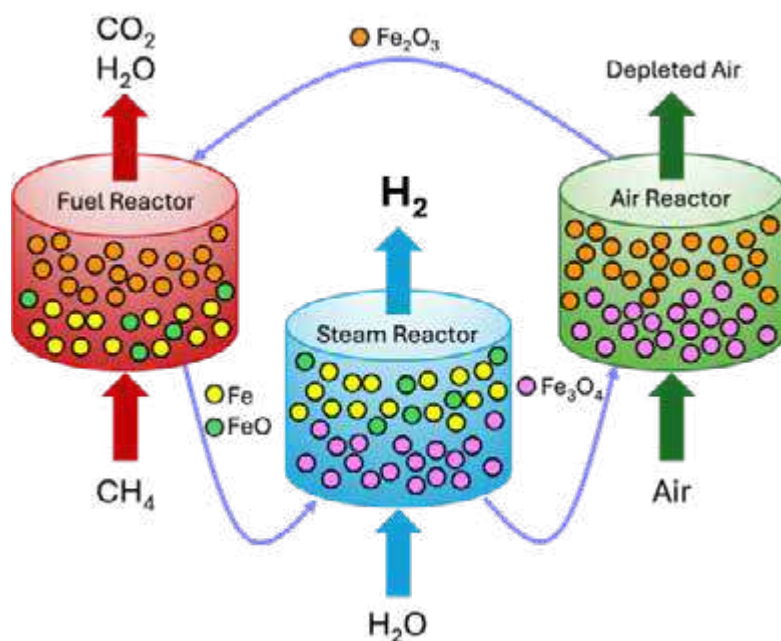
³Interdisciplinary Research Center for Hydrogen Technology and Carbon Management, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia

*Corresponding author: g202113590@kfupm.edu.sa

Abstract

Extensive research aims to enhance hydrogen production and reduce costs, mainly through blue hydrogen technologies as a transition technology. One promising innovation is chemical looping, which separates CO₂ during production without additional separation units. The effectiveness of this process relies on selecting the optimal oxygen carrier, with iron being a cost-effective and abundant option. This study investigates the impact of adding iron to a Ce-modified Al₂O₃ support in a fluidized bed reactor for hydrogen production. Research findings indicate that at a temperature of 650°C, F20Ce-Al demonstrates more potential for reduction to the iron state in fuel reactors compared to F30Ce-Al, primarily due to the involvement of the water-gas shift reaction (WGSR) in the reaction using F20Ce-Al. During the operation of the steam reactor, it was observed that F30Ce-Al exhibited the highest hydrogen production among the tested oxygen carriers within the first 5 to 16 seconds. However, beyond 16 seconds, hydrogen production decreased due to agglomeration of the oxygen carrier during the reaction process. In contrast, F20Ce-Al demonstrated the best performance in H₂ production compared to the other oxygen carriers.

Keywords: Blue hydrogen; Chemical looping; Oxygen carrier; Iron oxide; Fluidized bed



SULFONATED SOLID ACID CATALYST DERIVED FROM WASTE BANANA TRUNKS FOR BIODIESEL PRODUCTION STUDY

Shiau Huai Choong^{a*}, Chen Son Yue^a, Wai Suen Lim^a,

^a*Tunku Abdul Rahman University of Management and Technology, Malaysia.*

^{*}*Corresponding author: choongsh@taru.edu.my*

Abstract

The escalating global energy demand and environmental concerns have spurred the exploration of sustainable alternatives to traditional fossil fuels. This study investigates the potential of waste banana trunks, an abundant agricultural crop waste, in biodiesel production by synthesising sulfonated solid acid catalysts. This research encompasses synthesis processes including pyrolysis of waste banana trunks, sulfonation of solid acid catalysts, optimising preparation conditions, esterification of oleic and a comprehensive analysis of the catalysts' structural, thermal, and catalytic properties. The synthesised catalysts were characterised using Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TGA), and total acid density determination. The catalytic performance was evaluated through the esterification of oleic acid, revealing a maximum biodiesel yield of 21.05 % under optimised conditions. This study not only demonstrates the viability of utilising waste banana trunks for catalyst synthesis but also contributes to the development of sustainable and economically viable biodiesel production methods, offering a dual benefit of waste valorisation and renewable energy generation.

Keywords: waste banana trunks, biodiesel, sulfonated solid acid catalysts, esterification, renewable energy

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CARBON-NEUTRAL SOCIETY THAT CIRCULATES CARBON DIOXIDE AND METHANOL

Junji Nakamura

International Institute for Carbon-Neutral Energy Research, Kyushu University,

**Corresponding author: nakamura.junji.700@m.kyushu-u.ac.jp*

Abstract

Scientific research has confirmed that climate change is caused by anthropogenic CO₂ emissions. The rates of increase in annual primary energy consumption, annual CO₂ emissions, and atmospheric CO₂ concentrations correspond well. This is because primary energy is derived from fossil fuels and emits CO₂ as a result of combustion. Therefore, reducing CO₂ emissions is nothing less than energy revolution. To this end, large-scale renewable energy power generation is required, but the problem is energy storage and transportation. Batteries alone cannot solve the world's energy problems. It is absolutely necessary to convert electrical energy into liquid fuels that are easy to use around the world. The expected candidates are liquid hydrogen, ammonia, and methanol. We should discuss in detail and from various angles which substance to choose when aiming for carbon neutrality. In particular, chemists who synthesize these substances will be deeply involved in the energy problem. Among them, the most realistic substance is methanol. This conclusion is based on my 30 years of dedicated research on methanol synthesis catalysts from CO₂ [1-4]. Methanol can be used in internal combustion engines using existing technology and can be converted into electrical energy in fuel cells using methanol and hydrogen. Methanol can also be used to synthesize ethylene and propylene, which are raw materials for plastics. More importantly, it will enable us to build a recycling-oriented society that captures and effectively utilizes the CO₂ currently being emitted. Methanol is the only way to reduce CO₂ emissions quickly. In my presentation, I will talk about what we need to do to realize a methanol society. In particular, I will talk about energy efficiency, establishing a supply chain, creating a smart city, and citizen movements.

Keywords: Carbon neutrality, Methanol, catalyst, Cu/ZnO, CO₂

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OPTIMIZING TiO_2 PHOTOCATALYST WITH CO AND NI DOPING FOR IMPROVED HYDROGEN PRODUCTION

Hayyiratul Fatimah Mohd Zaid^{a,b,*}, Nur Ain Atiqah Mohd Amin^{a,b}

^a*Department of Chemical Engineering, Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak Darul Ridzuan, Malaysia*

^b*Centre of Innovative Nanostructures & Nanodevices (COINN), Universiti Teknologi PETRONAS, 32610 Seri Iskandar, Perak Darul Ridzuan, Malaysia.*

**Corresponding author: hayyiratul.mzaid@utp.edu.my*

Abstract

The demand for sustainable energy solutions has driven research into photocatalytic water splitting for hydrogen production. However, the low efficiency of photocatalysts under visible light remains a significant challenge. This study investigates the enhancement of TiO_2 photocatalysts through doping with cobalt (Co) and nickel (Ni), aiming to improve their hydrogen production efficiency under visible light irradiation. The main objective is to explore the effect of Co and Ni doping on the structural, optical, textural, and electrochemical properties of TiO_2 and their impact on photocatalytic hydrogen production. Co-Ni/ TiO_2 photocatalysts were synthesized via a sol-gel method and calcined under various conditions. The synthesized materials were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-Vis spectroscopy, Electrochemical Impedance Spectroscopy (EIS), Linear Sweep Voltammetry (LSV), and nitrogen adsorption-desorption analysis to assess their structural, morphological, optical, electrochemical, and textural properties. The results demonstrated that doping TiO_2 with Co and Ni significantly enhanced photocatalytic hydrogen production. The bimetallic Co-Ni/ TiO_2 photocatalyst achieved a maximum hydrogen production of 20.1 mL under optimized conditions. These conditions included: Co/ TiO_2 treated at 400°C for 2 hours with a 3.5 wt.% metal loading and a 1.0 g/L dosage; Ni/ TiO_2 treated at 500°C for 1 hour with a 5.0 wt.% metal loading and a 1.0 g/L dosage; and Co-Ni/ TiO_2 with a 2:1 Co:Ni mass ratio and a 1.25 g photocatalyst dosage. N_2 adsorption-desorption analysis confirmed that Co-Ni/ TiO_2 exhibited the highest surface area and porosity, enhancing active site availability and charge transfer. EIS analysis revealed reduced charge-transfer resistance, while LSV tests showed increased photocurrent density, indicating improved charge separation and mobility. In conclusion, Co and Ni doping effectively enhance the photocatalytic performance of TiO_2 , making it a promising material for hydrogen production under visible light. These findings provide valuable insights into optimizing photocatalysts for sustainable hydrogen production.

Keywords: Titanium dioxide; metal-doped; photocatalyst; photoelectrochemical cell; hydrogen production.



OPTIMIZING HYDRAULIC RETENTION TIME FOR ENHANCED BIOGAS AND METHANE PRODUCTION FROM ULTRASONICATED PALM OIL MILL EFFLUENT: A SUSTAINABLE APPROACH TO RENEWABLE ENERGY GENERATION

Lai Peng Wong^{a,*}, Wei Quan Law^a, Xinxin Guo^a, Mohammed J.K. Bashir^b

^a*Department of Environmental Engineering, Faculty of Engineering and Green Technology, Universiti Tunku Abdul Rahman, Jalan Universiti Bandar Barat, 31900 Kampar, Perak, Malaysia.*

^b*School of Engineering and Technology, CQUniversity Australia, L 3, 120 Spencer St, Melbourne Vic 3000, Australia.*

**Corresponding author: wonglp@utar.edu.my*

Abstract

Palm Oil Mill Effluent (POME) is an organic waste with a high concentration of Chemical Oxygen Demand (COD), necessitating treatment to minimize its environmental impact. Anaerobic digestion is an effective and cost-efficient method for POME treatment, offering the added benefit of biogas production, which can be harnessed as a renewable energy source. This study introduces ultrasonication pretreatment to enhance the efficiency of anaerobic digestion by breaking down complex organic compounds in POME, making them more accessible to microbial degradation. Additionally, the study focuses on optimizing Hydraulic Retention Time (HRT), a critical parameter influencing anaerobic digestion performance, to achieve higher biogas and methane yields while reducing operational costs.

A continuously stirred anaerobic bioreactor with a working volume of 250 mL was operated under ambient temperature and a mixing speed of 150 rpm. Ultrasonicated POME was fed into the reactor, and HRT values of 10, 8, and 7 days were evaluated. The results demonstrated that the reactor operating at a 7-day HRT achieved the highest biogas production of 577 mL/day and the highest methane yield of 0.226 mL CH₄/mg COD-digested, outperforming longer HRTs. This finding is significant as it demonstrates the potential to reduce operational costs without compromising treatment efficiency.

The integration of ultrasonication pretreatment with HRT optimization represents a novel contribution to POME treatment, offering a sustainable and scalable solution for palm oil mills. The increased biogas and methane production not only enhance the efficiency of the treatment process but also provide a renewable energy source that can offset the energy consumed during operations. This study highlights the potential of this approach to contribute to Sustainable Development Goal 7 (Affordable and Clean Energy) by transforming POME into a valuable energy resource while reducing its environmental impact.

Keywords: palm oil mill effluent (POME), anaerobic digestion, ultrasonication pretreatment, hydraulic retention time (HRT), biogas production

REVOLUTIONIZING DRY REFORMING OF METHANE WITH NICKEL-BIMETALLIC CATALYSTS ON DOLOMITE SUPPORT

Mohd Razali Shamsuddin^{a*}, Salma Samidin^b, Al-Sultan Kareem^c, Yun Hin Taufiq-Yap^c

^a *Preparatory Centre for Science and Technology, Universiti Malaysia Sabah, Jalan UMS, 88400 Kota Kinabalu, Sabah, Malaysia.*

^b *Department of Chemical and Process Engineering, Faculty of Engineering and Built Environmental Engineering, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia*

^c *Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia*

**Corresponding author: razalishamsuddin@ums.edu.my*

Abstract

The transition to a low-carbon economy is fraught with complexities, as methane and carbon dioxide, major contributors to global warming, can also serve as valuable feedstocks for syngas production through the dry reforming of methane. While touted as a promising solution for greenhouse gas mitigation and sustainable energy generation, dry reforming of methane remains hindered by a critical challenge: the rapid deactivation of nickel-based catalysts due to severe coke deposition. This study addresses this issue by developing nickel-based bimetallic catalysts supported on dolomite, incorporating iron, cobalt, molybdenum, and copper to enhance stability and performance. The Ni-X/Dol catalysts were synthesized using a wet impregnation method, leveraging the unique properties of dolomite to improve catalyst dispersion and durability. Comprehensive physicochemical characterization techniques, including X-ray diffraction, temperature-programmed desorption of CO₂, temperature-programmed reduction of CH₄, Brunauer-Emmett-Teller surface area analysis, and transmission electron microscopy, provided in-depth structural and surface insights. Catalytic performance tests revealed that bimetallic catalysts significantly outperformed their monometallic counterparts, achieving higher methane conversion and selectivity. Among them, Ni-Co/Dol demonstrated exceptional long-term stability with minimal coke formation, attributed to the synergistic effect of nickel and cobalt. These findings underscore the need for innovative catalyst designs to bridge the gap between DRM's theoretical potential and its industrial viability, offering a step toward more sustainable and energy-efficient syngas production.

Keywords: Dry reforming of methane; nickel; bimetallic; dolomite; catalyst

RECENT ADVANCES IN PHOTOCHARGEABLE MATERIALS FOR DARK PHOTOCATALYSIS

Wan Emilin Suliza Wan Abdul Rashid^a, Mohamad Azuwa Mohamed^{a,b,*}

^a *Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.*

^b *Fuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.*

**Corresponding author: mazuwa@ukm.edu.my*

Abstract

The urgent need for sustainable energy solutions has driven extensive research into semiconductor photocatalysis. While conventional photocatalysis offers a promising route for driving light-induced reactions, its reliance on continuous solar irradiation imposes significant limitations in terms of efficiency and scalability. To address this, dark photocatalysis has emerged as an alternative strategy that utilizes photochargeable materials capable of storing charge during daylight and releasing it in the dark, enabling photocatalytic reactions to proceed beyond light exposure. A critical factor in advancing dark photocatalysis is developing photochargeable photocatalysts that demonstrate enhanced charge separation and storage capabilities. Recently, significant effort has been focused on improving the charge storage properties of photocatalytic materials to boost reaction rates and enhance overall energy conversion efficiency under light-independent conditions. However, a comprehensive understanding of how material modifications influence the performance of photochargeable systems in dark photocatalysis is still lacking. This review highlights recent advances in the development and design of photochargeable materials specifically tailored for dark photocatalysis. Key classes of materials, including metal oxides, carbon-based frameworks, metal-organic frameworks (MOFs), and heterojunction structures, are discussed. By examining emerging material strategies, this work offers valuable perspectives on the current progress in dark photocatalysis and suggests future directions for continued advancement. Notably, these advancements support clean energy development and climate action efforts, aligning with the United Nations Sustainable Development Goals.

Keywords: dark photocatalysis, photochargeable materials, charge storage, sustainable energy

ENHANCING OPTIMIZATION OF FLOW CHANNEL DESIGN AND CONFIGURATION IN POLYMER ELECTROLYTE MEMBRANE FUEL CELL

Tan Kang Huai^{a*}, Kishore Rao A/L Bapu Naidu^a

^aCentre for Advanced Materials, Faculty of Engineering and Technology, Tunku Abdul Rahman University of Management and Technology, Jalan Genting Kelang, Setapak, 53300, Kuala Lumpur, Malaysia.

Abstract

The Performance of Polymer Electrolyte Membrane Fuel Cells (PEMFC) such as the temperature distribution, current output, and power output will be affected by a few factors. The design and configuration of current collector such as geometry design and number of flow channels play a crucial role in determining the efficiency, performance, and durability of the fuel cell. The aim of this study is to optimize the performance of PEMFC by determining the optimal number of flow channels and the best flow configuration. 8, 11, 15 channels were designed with various flow configurations such as co-flow, counter-flow and cross-flow and the study was carried out by using the Computer Fluid Dynamic simulation method. The materials for the electrolyte membrane and gas diffusion layer are Nafion and carbon paper. The effect of flow configuration on the temperature distribution 15 channel with cross-flow configuration obtained a better thermal performance because 15-channel with cross-flow has the lowest temperature difference of 0.048% compared to 8 and 11 channel. Moreover, 8 channels with counter-flow generates highest current density with 5582.330 A/m². However, the temperature contour is not the most uniform as compared to 11 and 15 channel. In conclusion, 11 channel with cross-flow configuration optimizes the performance with a promising electrical performance which shows maximum current density of 4103.920 A/m² and significant balance of temperature contour

Keywords: PEMFC, Computer Fluid Dynamic, Modelling, Current Collector

PEROVSKITE-BASED MATERIALS FOR PHOTOELECTROCHEMICAL GREEN AMMONIA

Nicola Sangiorgi ^{a*}, Alberto Soccio ^{a,b}, Alex Sangiorgi ^a, Alessandra Sanson ^a

^a *Institute of Science, Technology and Sustainability for Ceramics, National Research Council of Italy (CNR-ISSMC)*

^b *University of Parma, Department of Materials Science*

*Corresponding author: nicola.sangiorgi@issmc.cnr.it

Abstract

Solar fuels are synthetic fuels produced using solar energy. The primary energy source for these fuels is sunlight, which is converted into chemical energy stored in bonds, for example reducing protons to hydrogen, carbon dioxide to organic compounds or nitrogen into ammonia. Among them, the latter (N_2 RR) represents today one of the most attractive scientific and technological challenges to overcome in the energy field ¹. Solar fuels can be produced through various methods, including photochemical, photobiological, electrochemical, and thermochemical processes. Photo-electrochemical cell (PEC) represents one of the most interesting technologies for solar fuels production, and for this aim highly efficient and photo-active materials are required. Perovskite materials (ABO_3) and their layered structures, such as the double layered one, have been exploited for solar fuels production due to their low-cost, versatile structure, optical, electronic and photocatalytic properties. In this work, $CaCu_3Ti_4O_{12}$ (CCTO) due to its compositional variety was studied as photo-electrode material for PEC applications to reduce nitrogen into ammonia by N_2 RR. This oxide was synthesized by molten salt route and the structural (XRD), optical (band gap), and morphological characterizations on the obtained powders were carried out. The final materials were used to produce photo-electrodes with low costs and scalable solution-based processes; electrochemical and photo-electrochemical properties of these films were assessed by different techniques (cyclic and linear voltammetry, electrochemical impedance spectroscopy). The correlation between structural and functional properties was discussed highlighting the potentiality of this class of materials for solar energy conversion by photo-electrochemical cell technology.

Keywords: Photo-electrochemical cell, perovskite, green ammonia, photoelectrode, electrochemistry

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SOLAR AND LASER PHOTOACTIVATED MATERIALS FOR HIGH PERFORMANCE ENERGY STORAGE DEVICES

Weiping Wu^{a,*}

^aLaboratory of Thin Film Optics, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, 390 Qinghe Road, Jiading District, Shanghai 201800, China

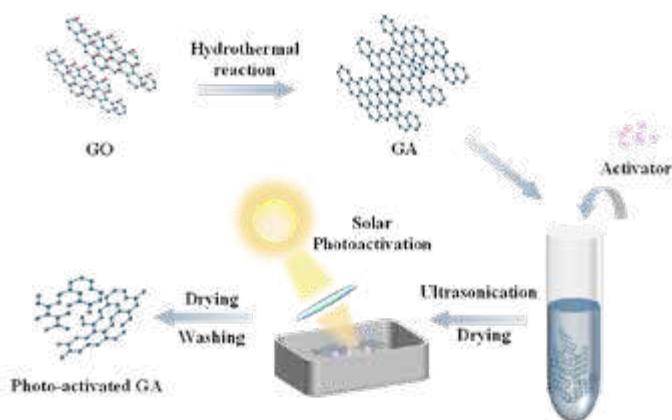
^aState Key Laboratory of High Field Laser Physics, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, 390 Qinghe Road, Jiading District, Shanghai, China

*Corresponding author: wuwp@siom.ac.cn

Abstract

Supercapacitors and batteries are emerging as promising energy storage devices. However, preparing high performance electrode materials with facile and low-energy processing remains a challenge. In this work, we introduce a novel photoactivation approach—using both solar and laser irradiation—to synthesis graphene aerogels and other materials for high-performance supercapacitor and battery applications. By employing a straightforward, cost-effective, and environmentally friendly process, nanoporous graphene aerogel “flowers” with an enhanced specific surface area were developed. This unique porous architecture significantly improves ion transport and charge storage efficiency, yielding a specific capacitance of up to 264 F/g. Moreover, the photoactivated electrodes demonstrate excellent cycling stability, retaining 80.9% of their initial capacitance after 10,000 cycles at a current density of 10 A/g. Compared to traditional high-energy activation methods, our photoactivation technique offers substantial advantages in terms of energy consumption and process simplicity, paving the way for scalable production of advanced electrode materials. This study highlights the potential of integrating solar and laser photoactivation methods to boost the performance of graphene-based supercapacitors, suggesting a promising direction for next-generation energy storage technologies.

Keywords: laser, solar energy, photoactivated materials, energy storage



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TRANSITION TO A CLEAN ENERGY FUTURE BY DECENTRALIZING HYDROGEN PRODUCTION

Joaquim L. Faria^{a,b*}, Manuel Peñas-Garzón^{a,b,c}, Goran Drazic^d,
Cláudia G. Silva^{a,b}, Maria J. Sampaio^{a,b}

^aLSRE – LCM – Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, Porto, 4200-465, Portugal

^bALiCE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, Porto, 4200-465, Portugal. *majsampaio@fe.up.pt

^cDepartamento de Ingeniería Química, Andalucía Tech, University of Málaga, Campus de Teatinos s/n, Málaga 29010, Spain

^dDepartment of Materials Chemistry, National Institute of Chemistry, Hajdrihova 19, Ljubljana, Slovenia

*Corresponding author: jlfaria@fe.up.pt

Abstract

Sustainable hydrogen production is key to the transition to a clean energy future. Following decades of cumulative research on the various aspects of photocatalytic and photoelectrochemical water splitting, the focus must be on minimizing environmental impact while ensuring efficiency and economic viability. On the one hand, the valorization of real urban wastewater (WW) for continuous hydrogen production via photocatalysis under visible light addresses the issue of genuinely sustainable production. However, the simple fact that we deal with a platinum-reduced photocatalyst requires adopting integrated circular economy models and securing strong policy support, which is critical for the large-scale implementation of decentralized production.

We seek a modular approach [1] using g-C₃N₄ based photocatalyst impregnated with 0.6% Pt as a co-catalyst immobilized on a polymeric film for H₂ production. This study evaluates the photocatalytic performance of powdered and immobilized Pt-g-C₃N₄ (Pt-CNX and Pt-CNX/F) for H₂ generation from real urban wastewater under visible light.

The immobilized Pt-CNX/F revealed comparable efficiency with powder photocatalyst, rendering a promising solution for sustainable H₂ generation, eliminating the need for reaction separation steps, enabling reutilization and facilitating continuous flow operation. Additionally, the Pt-CNX/F photocatalyst maintained its activity after reuse and facilitated easy recovery without compromising its photocatalytic performance when immobilized on a polymeric film. The organic pollutants naturally present in wastewater eliminate the need for sacrificial agents, enhancing H₂ production. This fact supports the effective valorisation of urban WW as a sustainable resource for photocatalytic H₂ generation under visible light.

Keywords: wastewater streams; continuous H₂ generation; photocatalysis; graphitic carbon nitride (g-C₃N₄); polymeric film

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THE ROLE OF P-BLOCK METAL ELEMENTS IN ELECTROCATALYTIC SULFUR OXIDATION: DESIGN OF BI-CuCoS_x/CF ACTIVE SITES

Shuai Li^a, Wenchao Peng^{a,b,*},

^a School of Chemical Engineering and Technology, Tianjin University.

^b Haihe Laboratory of Sustainable Chemical Transformations, Tianjin University.

*Corresponding author: wenchao.peng@tju.edu.cn

Abstract

This study proposes a new low-energy strategy for hydrogen production through electrolysis of water based on sulfur oxidation reaction (SOR) rather than traditional oxygen evolution reaction (OER). A copper cobalt based sulfide bifunctional catalyst (Bi-CuCoS_x/CF) controlled by bismuth metal element grown in situ on carbon felt (CF) was designed to effectively couple SOR and hydrogen evolution reaction (HER) in alkaline systems, addressing the problem of high water consumption in electrolysis caused by slow OER kinetics. Experiments have shown that at a current density of 100mA cm⁻², the catalyst only requires 0.48V (vs. RHE) to drive the entire reaction, which is about 73% lower than the voltage of traditional electrolysis water systems. The electronic structure reconstruction and nanocube structure characteristics caused by bismuth element were revealed through XRD, SEM, TEM, and XPS characterization. By combining in situ Raman spectroscopy, the dynamic evolution mechanism of active sulfur species during the SOR process was elucidated. The catalyst maintained a current efficiency of 91% during 100 hours of continuous operation, demonstrating excellent stability. This work provides a theoretical basis and examples for the development of low-cost, low-energy green hydrogen production technology through innovative reaction pathways and catalyst design.

Keywords: Sulfur oxidation reaction, electrocatalysis, bismuth doping, p-block element, Hydrogen evolution reaction

INTERFACIAL-ENGINEERED BIMETALLIC CATALYSTS FOR PHOTOTHERMAL CO HYDROGENATION

Zhaoda Xie^a, Tao Xie^{a,*}

^a Xi'an Jiaotong University.

*Corresponding author: xietao_xjtu@xjtu.edu.cn

Abstract

The direct conversion of carbon monoxide (CO) using green hydrogen presents a sustainable pathway for producing value-added liquid fuels. We have developed advanced carbon-supported catalysts to enhance Fischer-Tropsch synthesis (FTS) performance by modulating interfacial electronic structures and reaction pathways. Herein, discussion will focus on the following key achievements:

1. ZnCoFe@C catalyst for long-chain hydrocarbon selectivity¹
MOF-derived Zn₅CoFe₃₅@C catalyst was designed to regulate the Co–Fe electronic interaction, achieving a CO turnover yield of 739.3 mmol gcat^{−1} h^{−1} with 96.8% C₅₊ selectivity and minimal CH₄/CO₂ byproducts under mild conditions (350 °C, 0.1 Mpa).
2. Plasmonic CoRu@C catalyst for photothermal FTS²
Carbon-supported plasmonic CoRu₅@C catalyst enabled efficient C–C coupling under photothermal conditions (250 °C, 0.1 Mpa), delivering 98.9% C₅₊ selectivity and an activity of 321.4 mmol gcat^{−1} h^{−1} via strain-induced charge carrier migration and electron-rich Co sites.

These findings provide novel strategies for selective CO hydrogenation and sustainable fuel synthesis, advancing the design of high-performance catalysts for C₁ chemistry and renewable energy applications.

Keywords: Fischer-Tropsch synthesis, carbon-supported catalysts, plasmonic catalysis, interfacial electronic modulation, C–C coupling

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LOCAL-STRUCTURE AND CHEMICAL-ORDER MODULATION OF HEAS FOR ENHANCED OER PERFORMANCE

Xindong Zhu^a, He Zhu^{a,*},

^aNanjing University of Science and Technology, Nanjing 210094, China.

*Corresponding author: hezhu@njust.edu.cn

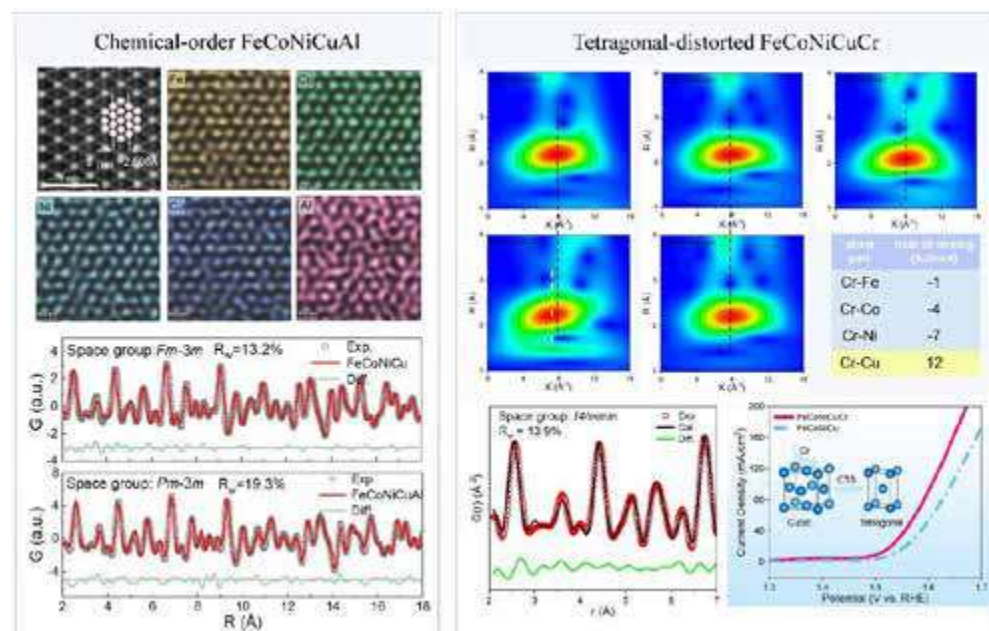
Abstract

High entropy alloys (HEAs) have become a next-generation electrocatalytic material due to their unique advantages, such as diverse active sites, a tunable and nearly continuous distribution of adsorption energy and significant potential for improving catalytic performance. However, HEAs are difficult to establish a correlation between structure and performance by modulating the structure due to the disorder of atomic arrangement and complex local structure. We have aimed at the development of efficient HEA electrocatalysts by introducing non-active elements such as Al and Cr, and explain the structure-activity relationship from a local structural perspective. Herein discussion will be focused on the following points with the goal of explaining the differences in the electrocatalytic performance of introducing different elements into HEAs.

1. Introducing Al to synthesize L_{12} nano multi principal element intermetallic compounds, long-range chemical ordering effectively isolates active sites and enhances OER activity. [1]
2. Incorporating Cr introduces local tetragonal distortions, attributed to atomic-scale elemental segregation between Cr and Cu, resulting in residual strain that enhances catalytic performance. [2]

As a result, our research validates that incorporating non-active elements into HEAs to modulate the structure is an effective approach for enhancing the performance, providing references for researchers exploring structure-performance relationships in HEAs.

Keywords: high entropy alloys, oxygen evolution reaction, local structural distortion, chemical-order modulation



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LOCAL ELECTRON BAND STRUCTURE REGULATION FACILITATES EFFICIENT PHOTO- THERMAL CATALYSIS OF CO₂ METHANATION OVER NI-CERIA CATALYST

Zhen-Yu Zhang^a, Tao Xie*,

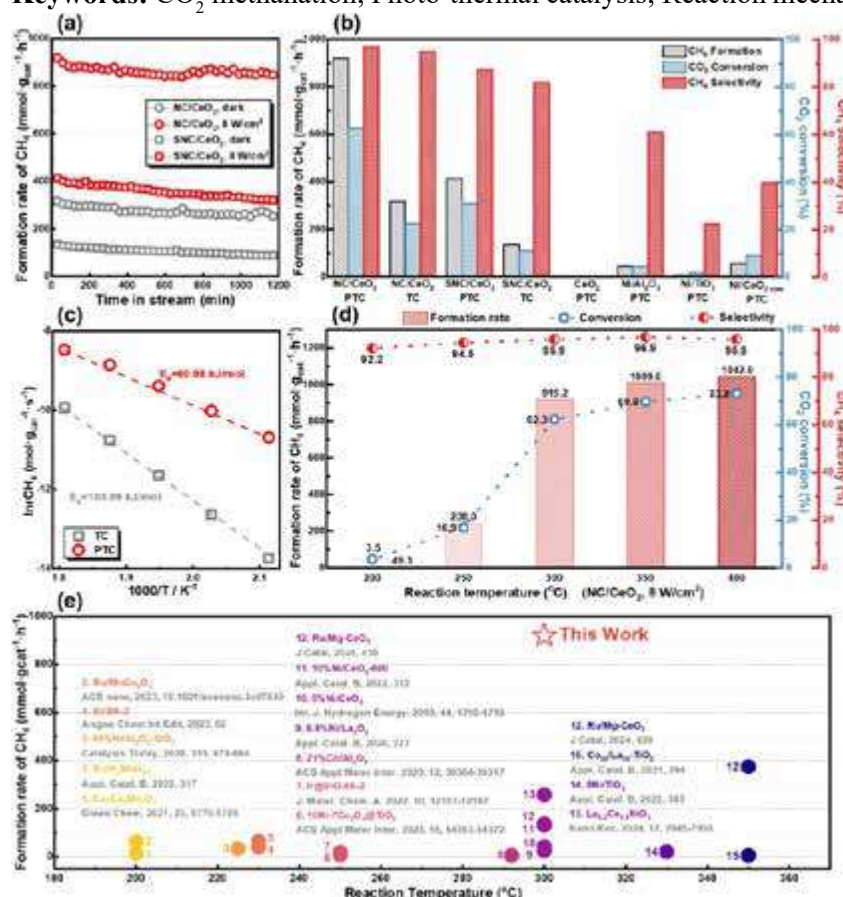
^a Institute of Industrial Catalysis, School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, PR China of author Zhen-Yu Zhang and Tao Xie

*Corresponding author: xietao_xjtu@xjtu.edu.cn

Abstract

Using solar energy to drive CO₂ methanation to eliminate carbon footprint is a very promising route. Through the photothermal synergistic effect, the reaction equilibrium limit can be approached at low temperature by breaking the “seesaw” effect of the reaction, with the help of further design of the catalyst. Here, based on the Ni-CeO₂ catalyst system, we fine-regulated the electronic band structure at the interface, and achieved a CO₂ conversion rate close to the thermal equilibrium limit and a CH₄ selectivity of > 97% under photothermal catalysis (PTC) conditions. At the same time, based on the fine structure characterization and theoretical calculation, the targeted transfer path from CO₂ to COOH* or HCOO* species was demonstrated. This work provides a theoretical basis for the subsequent optimization of the catalyst system.

Keywords: CO₂ methanation; Photo-thermal catalysis; Reaction mechanism; Ni-based catalyst



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SERPENTINIZATION-DRIVEN WHITE HYDROGEN PRODUCTION: A NATURE-INSPIRED APPROACH USING SYNTHETIC OLIVINE

Safyan Akram Khan^{a*} Muhammad Mansha^a Shahid Ali^a Sumaira Manzoor^a

^a *Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management*

King Fahd University of Petroleum and Minerals

**Corresponding author: safyan@kfupm.edu.sa*

Abstract

This study presents a nature-inspired strategy for sustainable white hydrogen production through the serpentinization of synthetic olivine, a process modelled after the natural geochemical transformation of ultramafic rocks. In geological settings, serpentinization is known to release molecular hydrogen as a byproduct of olivine reacting with water under elevated temperature and pressure. Building on this mechanism, we have engineered a synthetic olivine formulation optimized for controlled hydrogen generation under conditions analogous to those found in depleted geological reservoirs. Experimental investigations under hydrothermal conditions demonstrate the efficacy of our synthetic olivine in facilitating serpentinization-driven hydrogen evolution, with enhanced kinetics and yields. The process produces not only stable serpentine minerals but also generates a continuous flux of high-purity hydrogen. The synthetic formulation allows fine control over reaction parameters and scalability, making it suitable for in-situ hydrogen production in deep subsurface environments. This approach offers a clean, geologically-integrated solution for hydrogen generation without carbon emissions, utilizing existing depleted reservoirs as natural reactors. Our findings provide a promising pathway for large-scale, low-impact hydrogen production, contributing to the broader goals of sustainable energy transition and carbon-neutral fuel alternatives.

Keywords: Serpentinization, Olive, White Hydrogen, Reservoir

AMR CONTROL AND RESOURCE UTILIZATION OF LIVESTOCK MANURE THROUGH ANAEROBIC DIGESTION

Junya Zhang^{a,b}, Yuansong Wei^{a,b*}

^a State Key Laboratory of Regional Environment and Sustainability, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China.

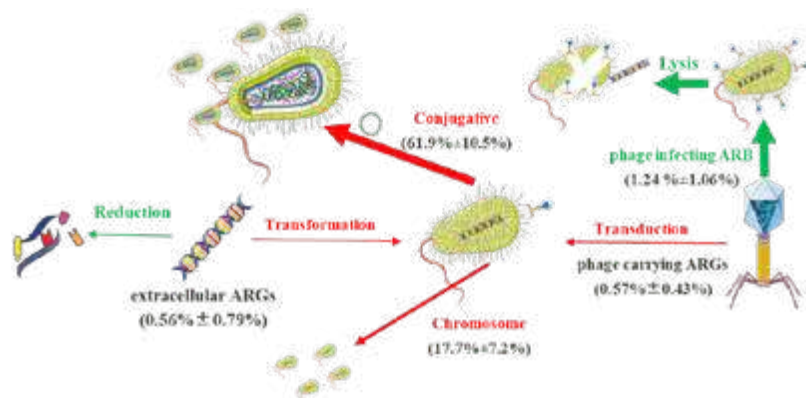
^b University of Chinese Academy of Sciences, Beijing 100049, China.

*Corresponding author: yswei@rcees.ac.cn

Abstract

Livestock manure, a major reservoir and source of antimicrobial resistance genes (ARGs), poses environmental and public health risks but also represents a valuable resource for energy and nutrient recovery. Anaerobic digestion (AD) is a widely adopted technology for the sustainable management of livestock manure, offering a dual benefit of resource utilization and potential AMR control. We aimed to enhance both AMR control and resource recovery by optimizing AD processes. Key research efforts and findings include: 1) Optimization of critical AD parameters, such as solids retention time (SRT), reactor configuration, temperature, and the addition of iron-based compounds, significantly improved methane production while simultaneously reducing ARG abundance. 2) We identified key factors influencing AMR control during AD and elucidated the fate of intracellular, extracellular, and phage-mediated ARGs. 3) Notably, phage-mediated ARG reduction was found to be substantially greater than dissemination, highlighting the potential of phages in mitigating AMR spread. Based on this, a novel phage-targeted AMR control strategy was proposed to further enhance the efficacy of AD in reducing ARG prevalence. These findings underscore the potential of optimized AD processes to achieve synergistic benefits in AMR mitigation and resource recovery. By integrating advanced process control and phage-based strategies, this approach provides a sustainable framework for managing livestock manure, reducing environmental AMR risks, and promoting renewable energy production, thus contributing to both agricultural sustainability and public health protection.

Keywords: Antimicrobial resistance genes; Livestock manure; Anaerobic digestion; Viral community; Methane production



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DEVELOPMENT AND CHARACTERIZATION OF SCSZ-SDC COMPOSITE CATHODES FOR INTERMEDIATE-TEMPERATURE SOLID OXIDE FUEL CELLS

Nurul Farhana Bt Abdul Rahman^a, Sheikh Ahmad Safwan Bin Shaikh Sabri^a,
Umira Asyikin Bt Md Yusup^a, Hamimah Bt Abd. Rahman^a, Tan Kang Huai^b

^aFaculty of Mechanical Engineering, Universiti Tun Hussein Onn Malaysia

^bCentre for Advanced Materials, Faculty of Engineering and Technology Tunku Abdul Rahman University of Management and Technology.

*Corresponding author: tankanghuai@taru.edu.my

Abstract

The excellent ionic conductivity and stability of samarium-doped ceria (SDC) and Scandia-stabilized zirconia (ScSZ) materials captured significant interest in the capacity to operate at lowered temperatures. In this study, a composite cathode comprising scandia-stabilized zirconia (ScSZ) and samarium-doped ceria (SDC) was synthesized via the wet ball milling method for intermediate-temperature solid oxide fuel cells (IT-SOFCs). ScSZ-SDC composite powders were prepared in five different compositions with the weight ratios 50-90ScSZ:50-10SDC (ScSZ-SDC), followed by a calcination process. The analysis of the prepared powders included an examination of chemical compatibility, structural, and morphological properties. X-ray Diffraction (XRD) was employed to determine phase compatibility between ScSZ and SDC materials, Field Emission Scanning Electron Microscopy (FESEM) was utilized to examine the microstructure of the developed composite powders, and Energy-Dispersive X-ray Spectroscopy (EDS) was applied to assess the elemental distribution within the ScSZ-SDC composite powders. Subsequently, the calcined powders were compacted into pellets using the uniaxial pressing method to ensure mechanical integrity and uniform density of the samples. The fabricated pellets were evaluated using electrochemical impedance spectroscopy (EIS) testing at firing temperatures of 800°C, 700°C, and 600°C to assess the ionic conductivity and overall electrochemical performance. Furthermore, porosity testing was conducted to analyse the influence of porosity on the electrochemical properties and to refine the composite formulation. This study provides significant insights into the relationship between composition, microstructure, and electrochemical performance of ScSZ-SDC composite cathodes across the five compositions examined. The results advance the creation of effective and stable cathode materials for IT-SOFC applications, highlighting the necessity of optimizing material composition and processing methods.

Keywords: Composite Cathodes, ScSZ, SDC, Solid Oxide Fuel Cell

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BIODIESEL ADDITIVE FORMULATION AND ITS APPLICATION

Noor Fitri^{1,2 *}, Khofifah¹, Irfan Aditya Dharma³, Nurcahyo Iman Prakoso^{1,2}, Qomarudin Sukri⁴

¹Master of Chemistry, Universitas Islam Indonesia

²Center of Essential Oil Study, Chemistry Department, Universitas Islam Indonesia

³Department of Mechanical Engineering, Universitas Islam Indonesia

⁴PT. Arutmin Indonesia Tambang Kintap, Kalimantan Selatan

* Corresponding author: noor.fitri@uii.ac.id

Abstract

Indonesia's transportation sector is among the largest fuel consumers, with fuel usage increasing by approximately 4% annually. To reduce reliance on petroleum-based fuels, sustainable alternatives like biofuels and natural additives are being explored. This study investigates the impact of adding bio-additives on the quality of B35 biodiesel. The research includes: 1) GC-MS analysis of both biodiesel and bio-additives; 2) Formulation of the bio-additives; 3) Blending of B35 with bio-additives; 4) Characterization of the blended fuel; and 5) Testing the performance of B35 with bio-additives in laboratory settings, as well as in medium and heavy diesel engines. The findings indicate that the main fractions of citronellal, rhodinol, and alpha-pinene demonstrated the highest efficiency across all testing platforms. Among them, citronellal was most effective at reducing HC and CO₂ emissions during laboratory-scale emission tests.

Keywords: biodiesel B35; bio-additives; citronellal; rhodinol; alpha-pinene

ENGINEERING NANOCATALYSTS FOR HYDROGEN EVOLUTION: A FOCUS ON STRUCTURE–ACTIVITY RELATIONSHIPS

Nosipho Moloto^{*}, Siyabonga Nkabinde^b, Zakhele Ndala^b, Lineo Mxakaza, Victor Mashindi

^a*School of Chemistry, University of the Witwatersrand, P. O. Box 2050, Johannesburg 2000*

^{*}*Corresponding author: Nosipho.Moloto@wits.ac.za*

Abstract

The development of efficient, cost-effective nanocatalysts is critical to advancing hydrogen evolution reaction (HER) technologies for sustainable energy systems. This work explores the rational design, synthesis, and characterization of nanostructured catalysts tailored for enhanced HER performance. Emphasis is placed on correlating structural and compositional features with catalytic activity, including crystallinity, morphology, electronic structure, and surface chemistry. Advanced techniques such as XPS, EXAFS, PDF and electrochemical measurements are employed to elucidate these structure–activity relationships. The findings provide insights into the role of synergistic interactions, offering pathways for the optimization of next generation HER catalysts.

Keywords: Hydrogen Evolution Reaction (HER); Nanocatalysts; Electrocatalysis

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RISING TO CHALLENGE: HARNESSING CHEMISTRY FOR CLIMATE ACTION AND SUSTAINABLE FUTURE

Elizabeth Philip

Forest Research Institute Malaysia (FRIM) 52109 Kepong, Selangor.

**Corresponding author: philip@frim.gov.my*

Abstract

Climate change is no longer a distant concern—it is a present reality, marked by rising global temperatures, extreme weather, and disrupted ecosystems. In response, Sustainable Development Goal 13, set by the United Nations in 2015, emphasizes urgent and transformative action to combat climate change. One of the most powerful tools in this fight is chemistry. Chemistry plays a crucial role in understanding and addressing climate change by shedding light on key processes like greenhouse gas emissions, the carbon cycle, and atmospheric reactions. It helps identify and quantify greenhouse gases (CO_2 , CH_4 , N_2O), assess carbon storage and release due to human activities, and predict climate impacts through atmospheric chemistry. Additionally, chemistry aids in developing climate models that simulate future scenarios and inform policy decisions. Beyond understanding climate change, chemistry drives innovative solutions. It fuels renewable energy advancements such as next-generation solar panels, hydrogen fuel cells, and energy-dense batteries that stabilize grids by storing clean energy. Furthermore, chemical processes support carbon capture, utilization, and storage (CCUS) technologies, converting carbon emissions into valuable resources like fuels and building materials. Green chemistry pushes sustainability further by designing eco-friendly products and processes. It promotes biodegradable plastics, non-toxic chemical alternatives, and sustainable farming practices that reduce carbon footprints. Innovations in chemical recycling are advancing circular economies by repurposing waste materials rather than polluting ecosystems. Chemistry also strengthens forest climate strategies by monitoring carbon sequestration, analysing soil fertility, and assessing forest health. Understanding wildfire chemistry aids in developing better fire retardants and treatments to combat increasingly intense fires. Ultimately, combating climate change requires collaboration between science, policy, and industry. When chemists, policymakers, and businesses work together, they drive impactful innovations like renewable fuels, plastic recycling, and energy-efficient processes—crucial to reducing greenhouse gas emissions and conserving natural resources. Chemistry is a catalyst for a sustainable future.

Keywords: climate change solutions chemistry

LIFE CYCLE THINKING IN CHEMICAL STEWARDSHIP

Chan Kok Meng^{a,*}, Salmaan Hussain Inayat-Hussain^b

^a*Petroleum Nasional Berhad (PETRONAS)*

^b*Ipieca*

**Corresponding author: chan.kokmeng@petronas.com*

Abstract

Chemical stewardship is key in managing chemical safety through a sound management of chemicals throughout their lifecycle. This is to ensure that chemicals are produced and used in ways that minimize significant adverse impacts on human health and environment. This is aligned with the UN Sustainable Development Goals (SDGs), the world's comprehensive plan of action, which includes goals to ensure good health and well-being, responsible consumption and production and climate action. From the 17 SDGs, there are 4 SDGs with specific targets which are directly linked to chemicals and waste management. For example, under SDG Goal 3, Target 3.9 is on the reduction of the number of deaths and illnesses from hazardous chemicals by 2030 and Goal 6 has a target to improve water quality by reducing pollution of chemicals. Target 12.4 is very important as it is to achieve the environmentally sound management of chemicals and waste throughout the life cycle, and we have under SDG 13 on climate action. In order to achieve these goals, industries need to integrate chemical stewardship to protect workers and community members against adverse health outcomes from chemical exposure and climate change. This talk will discuss the interdisciplinary approaches in addressing chemical stewardship throughout the life cycle of chemicals.

Keywords: Chemical Stewardship, Life Cycle, Sound Chemical Management

PEAT SWAMP FOREST AS AN IMPORTANT CARBON SINK AND SOURCE IN CLIMATE CHANGE MITIGATION

Jeyanny Vijayanathan^{a*}, Mohamad Fakhri Ishak^a, Siti Aisah Shamsuddin^b, Muhammad Asri Lias^a
& Mohd Syamin Mohd Aizat^a,

^aForest Plantation Programme, Forest Biotechnology Division, Forest Research Institute Malaysia, 52109 Kepong Selangor.

^aClimate Change & Environment Programme, Forestry & Environment Division, Forest Research Institute Malaysia, 52109 Kepong Selangor.

*Corresponding author: jeyanny@frim.gov.my

Abstract

Peat swamp forests play a vital role in regulating the global carbon cycle, as they act as carbon sinks by storing large amounts of carbon. They also provide habitat for a wide range of biodiversity, including many rare and endangered species. These forests are essential to local hydrology, filtering water, and preventing flooding, while also supporting traditional livelihoods. Ayer Hitam Utara Forest Reserve (AHFR) is located in the Muar district, Johor (1° 52' North, 103° 11' East) of Peninsular Malaysia. This area is known to be the largest and last peat swamp forest that covers around 3,797 hectares (ha). A preliminary investigation was done to determine the peat carbon stocks and the peat carbon fluxes of the area for carbon budget accounting. Soil samples were taken at 6 points in Compartment 14 for bulk density measurements at 0-15 and 15-30 cm depths and additional samples taken for C analysis in the laboratory. Soil CO₂ fluxes were measured using the Li-8100 automated soil CO₂ flux system at different intervals from August 2023 to December 2024. The area consists of very deep peat with dominance of hemic material. Results revealed that carbon stock values at 30 cm depth (279.45 tC ha⁻¹) were slightly higher than Pekan, Pahang PSF which reported values at 245 tC ha⁻¹ in 2015 (Parlan, 2017). Soil CO₂ fluxes ranged between 24.0 to 96.85 tCO₂ha⁻¹yr⁻¹ which was slightly higher for a peat swamp forest compared to Vijayanathan et al., (2021). This preliminary information on stocks and fluxes may serve as a pre-requisite for evaluating the AHFR for carbon credits and REDD+ financial mechanism.

Keywords: peat chemistry, wetlands; tropics; carbon balance; changing climate

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ULTRASOUND-ASSISTED SOLVO-HYDROTHERMAL SYNTHESIS OF CHITOSAN-LIGNIN COMPOSITES FOR EFFICIENT SELECTIVE OXIDATION OF MODEL LIGNIN COMPOUND BY SYNERGISTIC SONOPHOTOCATALYSIS

Juan Carlos Colmenares ^{*a}, Ahmed Malek Djaballah ^a, Behdokht Hashemi Hosseini ^a

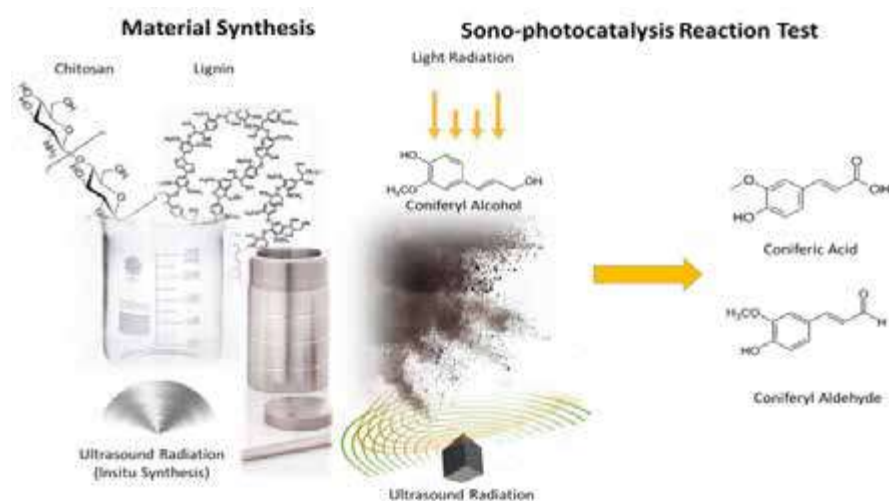
^aInstitute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

^{*}Corresponding author: jcarloscolmenares@ichf.edu.pl

Abstract

This study focuses on optimizing a solvo-hydrothermal process with ultrasonic assistance for synthesizing carbon-based materials and enhancing the selective oxidation of coniferyl alcohol (ConOH) into ferulic acid [1]. The influence of ultrasound parameters on the morphology, yield, and selectivity of chitosan/lignin (C/L) composites was evaluated. Structural and morphological analyzes (XPS, FTIR, SEM) confirmed the successful synthesis and stability of the materials under visible light irradiation in acetonitrile. Additionally, the incorporation of copper into the C/L matrix, validated by structural analysis, significantly enhanced oxidation performance by boosting (sono) photocatalytic activity and promoting selective reaction pathways. This study highlights the potential of ultrasound-assisted techniques for developing chitosan-lignin composites and underscores the synergistic role of Cu integration via photo-deposition, enabling efficient and eco-friendly biomass valorization into high-value aromatic compounds [2].

Keywords: Ultrasound-assisted synthesis, Chitosan-lignin composites, Selective oxidation, Photocatalysis, Biomass valorization



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3. This study was financially supported by the National Science Centre: in Poland under the **OPUS 20** research project **No. 2020/39/B/ST5/00076**.

EARTH-ABUNDANT ALUMINUM FORMATE (ALF) AS A SUSTAINABLE DECARBONIZATION SOLUTION: A MULTISCALE COMPUTATIONAL STUDY USING DFT, MD AND MC SIMULATIONS

Fouzia Perveen^{a,*}, Hadiqa Naaz^a

^a*School of Interdisciplinary Engineering & Science (SINES), National University of Sciences and Technology (NUST), H-12, Islamabad, 44000, Pakistan.*

**Corresponding author: fouzia@sines.nust.edu.pk*

Abstract

The increasing levels of atmospheric CO₂, driven by anthropogenic activities, have intensified the global climate crisis necessitating the urgent development of sustainable and efficient carbon capture technologies. In response, this study investigated Aluminum Formate (ALF), an earth-abundant metal-organic framework (MOF), as a highly promising material for CO₂ capture and decarbonization. To comprehensively evaluate ALF's potential, a multidisciplinary computational approach was employed, integrating Density Functional Theory (DFT), Molecular Dynamics (MD) and Monte Carlo (MC) simulations. DFT calculations revealed a direct bandgap of 5.295 eV, confirming ALF's electronic stability and suitability for adsorption applications, while Radial Distribution Function (RDF) analysis further demonstrated its highly ordered crystalline structure, underscoring its potential for efficient CO₂ capture. Building on these findings, MD simulations were conducted to assess ALF's thermal stability, revealing structural resilience up to 450 °C, a critical attribute for industrial applications. To evaluate ALF's CO₂ adsorption performance, MC simulations were performed, demonstrating a strong adsorption energy of -32.916 kcal/mol driven primarily by electrostatic interactions with Al-OH functional groups. These simulations also highlighted ALF's exceptional selectivity for CO₂ over nitrogen (N₂) and water (H₂O), with adsorption energies of -8.00 kcal/mol and -5.845 kcal/mol, respectively, positioning it as a superior candidate for selective gas separation. Comparative analysis with conventional adsorbents, such as zeolites, activated carbon, and amine-based sorbents, further revealed ALF's superior adsorption performance, thermal stability, and moisture resistance. Additionally, ALF's low-cost synthesis, scalability, and minimal environmental impact make it a viable candidate for large-scale industrial carbon capture. This research aligns with global sustainability goals, particularly the United Nations Sustainable Development Goals (SDG 13: Climate Action and SDG 9: Industry, Innovation, and Infrastructure), emphasizing the transformative role of advanced materials in addressing environmental challenges. By integrating DFT, MD and MC simulations, this study provides a robust understanding of ALF's stability and adsorption capabilities, establishing it as a cost-effective, sustainable, and scalable solution for CO₂ capture. These findings represent a significant advancement in the development of innovative carbon capture technologies, offering a promising pathway to mitigate climate change and achieve a sustainable, low-carbon future.

Keywords: Carbon Capture and Storage (CCS), Metal-Organic Frameworks (MOFs), Aluminum Formate (ALF), CO₂ Adsorption, Sustainable Decarbonization

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ATMOSPHERIC CHEMISTRY PREDICTION INITIATIVES IN MALAYSIA

Maggie Chel Gee Ooi^{a,*}, Nur Nazmi Liyana binti Mohd Napi^a, Liew Juneng^b, Mohd Talib Latif^b

^a*Centre of Tropical Climate Change System, Institute of Climate Change, Universiti Kebangsaan Malaysia (UKM), 43600 Bangi, Selangor*

^b*Department of Earth and Environmental Science, Universiti Kebangsaan Malaysia (UKM), 43600 Bangi, Selangor*

**Corresponding author: chelgee.ooi@ukm.edu.my*

Abstract

Air pollution is one of the prominent environmental issues in Malaysia, and both short-term and prolonged exposure have significant negative impacts on human health, including respiratory complications, cardiovascular problems, and even premature death. The atmospheric chemistry in the wet, tropical Malaysia has a higher tendency to form hydroxyl radicals, a highly reactive oxygen species. The country's emission profile is also complex due to anthropogenic emissions from rapid industrialization and growth, biogenic emissions from its vast coverage of forests and vegetation, and recurring haze from wildfire burning. To address this, the numerical chemical weather prediction offers a solution for accounting for the collective presence of multiple pollutants, weather-chemistry interactions and chemical processes. The work aims to present several initiatives undertaken to form the basis of the air quality prediction system that can accurately capture occurrences and estimate pollution level during haze period caused by burning. This includes the fine-tuning of the fire emission inventory, assimilating weather conditions, and developing a plume rise model. The ability to predict air quality is crucial for data-driven decision-making support for air quality management in Malaysia.

Keywords: PM_{2.5}, O₃, biomass burning haze, air quality modelling, WRF-CMAQ

SYNTHESIS OF CELLULOSE TRIACETATE FROM MILLET HUSK CELLULOSE: COMPARISON OF CHEMICAL AND ELECTROCHEMICAL METHODS

Maryam Khadim MBACKE^{a,*}, EL HADJ Moussa Diop^{b,c}, Mouhamed Ndoeye^c, Cheikhou Kane^c,

^a Laboratory of Sciences, Advanced Technologies and Sustainable Development (LSTADD), Amadou Mahtar Mbow University, Dakar, Senegal.

^b School of Industrial and Biological Engineering (ESGIB), Dakar, Senegal.

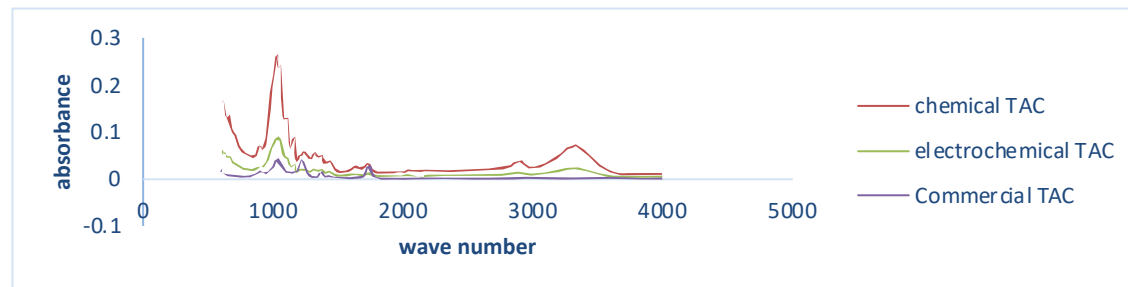
^c Laboratory of Water, Energy, Environment and Industrial Processes (LE3PI), Polytechnic School, Cheikh Anta Diop University, BP 5085, Dakar, Senegal.

*Corresponding author: maryam.mbacke@uam.edu.sn

Abstract

In a sustainable development perspective, lignocellulosic resources are increasingly valued in the field of membrane production as an alternative to petroleum-based raw materials [1]. In this study, cellulose triacetate (TAC) was synthesized from millet husk for future application in the production of nanofiltration membranes [2] [3]. After optimization of the cellulose extraction process, acetylation was carried out by chemical and electrochemical means. The results obtained showed respective degrees of substitution of 2.67 for the chemical method and 2.8 for the electrochemical method. The acetylation yields are 87.4 and 83.2% for the chemical and electrochemical methods, respectively. The TAC obtained was characterized by Fourier transform infrared spectroscopy analysis, X-ray diffraction and scanning electron microscopy. Thermogravimetric analysis was used to measure the thermal stability of the different products [4]. TAC was compared to a commercially available derivative. Acetylation by electrochemical method was shown to be a promising alternative to overcome the constraint of using large quantities of chemicals for the treatment of bio-based products.

Keywords: cellulose, husk, triacetate



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SUSTAINABLE SOLID WASTE MANAGEMENT WITH ONLINE SELF-REGULATED LEARNING AMONG PRIMARY SCHOOL STUDENTS

Nilavathi Balasundram^{a,*}, Punitha a/p Muniandy@Karthigasoo^b,
Muhd Ibrahim bin Muhamad Damanhuri, Mageswary a/p Karpudewan^c,

^aUniversiti Pendidikan Sultan Idris.

^bIPG Kampus Tuanku Bainun.

^cUniversiti Pendidikan Sultan Idris.

^dUniversiti Sains Malaysia

*Corresponding author: b.nilavathi@fsmt.upsi.edu.my

Abstract

Environmental education in recent years has been taught in the science education in most of the developing countries including Malaysia (Yaacob et al., 2019). Education on sustainable solid waste management (SWM) is an essential part of environmental education that need to be focussed due to the increasing volume of solid produced from various fields in every consequent year. Improper disposal of solid waste causes diverse environmental, social, economic and public health impacts (Raphela et al., 2024; Asfaw et al., 2024). However, the knowledge and the practical on sustainable SWM among students from primary to university level and teachers in many developing countries remains at minimal level (Fadhullah et al., 2022). Therefore, introducing SWM education at the primary level is crucial to instil proper disposal habits at early age contributing for sustainable future. This study integrates SWM in a science topic, waste materials in Year 6 syllabus. Year 6 students should be exposed to in-depth understanding about sustainable SWM which is in line with Sustainable Development Goal, SDG (2023) focussing on goal 12 (Responsible consumption and production) and goal 13 (Climate action). This study employs embedded mixed method research in which quantitative data is complemented by qualitative data. Primary students (12 years old) and primary school pre-service teachers took part in this study using an online interactive module produced using Genially software. Questionnaires and interview sessions were used to understand primary school students' and teachers' knowledge and practices before and after using the online interactive module towards sustainable solid waste management. The study indicates students demonstrate improved knowledge towards sustainable SWM and able to apply the knowledge in practice extending the impact to those around them.

Keywords: Sustainability, solid waste management, online, self-regulated learning, primary students

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APPLYING SYSTEMS THINKING AND SUSTAINABILITY IN HIGH SCHOOL RESEARCH: INVESTIGATING THE MEDICINAL POTENTIAL OF *FICUS RACEMOSA* LEAF GALLS

Chi Thanh Tran^{a,*}, Thanh Tai Vo^b, Thuy Ngoc Pham^c

^{a,b,c} Luong Van Can High School, District 8, Ho Chi Minh City, Vietnam

*Corresponding author: tranchithanh.lvc@gmail.com

Abstract

Merging *Systems Thinking* into chemistry education enhances students' understanding of sustainability. This study explores the medicinal properties of *Ficus racemosa* leaf galls, which form in response to *Psyllidae* insect infestations. These galls accumulate bioactive compounds, including gallic acid, traditionally used in Vietnamese medicine for wound healing. This research integrates *Green Chemistry* principles to support sustainable drug discovery. The analysis of *Ficus racemosa* leaf galls using qualitative methods identified the presence of multiple phenolic compounds. Due to the high phenol content, a recrystallization process was performed, yielding a pure white crystalline compound. This compound was characterized using thin-layer chromatography (TLC) and nuclear magnetic resonance spectroscopy (¹H NMR, ¹³C NMR). Biological assays evaluated fibroblast cytotoxicity, DPPH radical scavenging activity, Hep-G2 cytotoxicity, and α -glucosidase inhibition.

1. Antioxidant activity on DPPH radical: The SC₅₀ values of *Ficus racemosa* leaf gall extracts were as follows: ethanol extract 23.84 ± 2.16, gallic acid 1.29 ± 0.14, and the positive control Trolox 8.19 ± 0.21. Thus, gallic acid exhibited 6.3 times stronger antioxidant activity than Trolox.
2. Cytotoxicity on Hep-G2 cells: The ethanol extract of *Ficus racemosa* leaf galls inhibited 98% of Hep-G2 cells, with gallic acid showing an IC₅₀ = 5.09 ± 0.17.
3. Cytotoxicity on fibroblast cells: Gallic acid had minimal effects on fibroblast cells, with IC₅₀ = 10.48 ± 0.67, indicating low toxicity.
4. α -Glucosidase inhibition: The ethanol extract had an IC₅₀ = 13.2, while gallic acid had an IC₅₀ = 3.0. The positive control Acarbose had IC₅₀ = 138.1 and 214.3. Thus, gallic acid was 72 times more effective than Acarbose.

The results confirm that *Ficus racemosa* galls are an affordable, widely available natural resource with potential for sustainable healthcare applications. Integrating *Systems Thinking* and *Green Chemistry* into high school education fosters a sustainable learning model, combining traditional medicine with modern science to develop eco-friendly medicinal solutions.

Keywords: *Systems Thinking, Green Chemistry, Sustainability, High School Chemistry, *Ficus racemosa*



Table 1: DPPH Scavenging Activity (SC50 Values)

Sample	SC50 (µg/mL)			Average ± SD
	Test 1	Test 2	Test 3	
Trolox	8.45	8.11	8.06	8.19 ± 0.21
Gallic Acid	1.12	1.26	1.42	1.29 ± 0.14
EtOH Extract	21.82	23.58	26.12	23.84 ± 2.16

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ELECTROCHEMICAL CO₂ CONVERSION TO C₂ PRODUCTS: INFLUENCE OF CATALYSTS AND ELECTROLYZER DESIGN ON CURRENT DENSITY AND SELECTIVITY

Muhammad Usman^{a,*}, Munzir H Suliman^a, Naimat Ullah^a,

^aInterdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM),
King Fahd University of Petroleum & Minerals (KFUPM), Dhahran 31261, Saudi Arabia

*Corresponding author: muhammadu@kfupm.edu.sa

Abstract

The increase in atmospheric carbon dioxide (CO₂) concentrations, already over 420 ppm, presents a substantial risk to ecosystems worldwide. Researchers are investigating novel strategies within the circular carbon economy to mitigate this dilemma by emphasizing the reduction, reuse, removal, and recycling of CO₂. The electrocatalytic reduction of CO₂ (eCO₂RR), facilitating the transformation of CO₂ into useful products, is significantly affected by the selection of catalysts and the design of the electrolyzer. This research investigates the use of silver (Ag), zinc (Zn), and Copper (Cu) catalysts for the transformation of CO₂ into C₂ products, mainly ethylene (C₂H₄) and ethanol (C₂H₅OH). The efficacy of H-type and flow cells, which include distinct combinations of electrolytes and catalysts, is also assessed. Although H-cells are proficient for examining and representing the inherent catalytic characteristics of materials, flow cells exhibit superior current densities, underscoring their commercialization potential.

Keywords: CO₂ conversion, H cell, Flow cell, Electrocatalysts, Climate Action

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ENHANCING GAS SEPARATION PERFORMANCE IN PSF/ZTC MIXED MATRIX MEMBRANES THROUGH HEAT TREATMENT

Rika Wijiyanti^{a*}, Irmariza Shafitri Caralin^b, Alvin Rahmad Widyanto^c, Nurul Widiastuti^d

^a Medical Intelligence Postgraduate Program, Sekolah Tinggi Intelijen Negara (State Intelligence College), Sumur Batu, Babakan Madang, Bogor, 16810, Indonesia

^b Department of Regional Environment Systems, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan

^c Department of Applied Chemistry, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan

^d Department of Chemistry, Faculty of Science and Data Analytics, Institut Teknologi Sepuluh Nopember, Jl. Arif Rahman Hakim, Kampus ITS Keputih-Sukolilo, Surabaya, 60111, Indonesia

*Corresponding author: wijiyantirika@gmail.com

Abstract

The separation of gases into their individual components is essential for various industrial processes, including natural gas sweetening, carbon dioxide removal, and nitrogen or oxygen enrichment ¹. The use of membranes for gas separation is a rapidly emerging field due to their simplicity, low cost, high separation and energy efficiency compared to traditional methods ². This study introduces a newly engineered filler membrane, called zeolite templated carbon (ZTC), which is designed for superior gas separation performance. The large surface area and well-defined pore structure of ZTC enable effective separation in mixed matrix membranes (MMMs) ^{3,4}. ZTC was prepared by using a synthesized zeolite-Y template and a sucrose carbon source through the impregnation method. The MMMs were then fabricated using a dry-jet wet spinning technique, with ZTC loading varying between 0.25 and 0.5 wt%. However, avoiding interfacial voids in the MMMs proved challenging, leading to poor separation performance ³. This research aims to enhance separation performance by modifying the surfaces of the membranes. The MMM PSF/ZTC was altered by heating at 200°C for 30, 120 and 240 minutes. Notably, the MMM with 0.25wt% ZTC loading exhibited significant improvement in gas selectivities after 240 minutes of heating: CO₂/CH₄ selectivity increased from 5.28 to 39.65 (651%), O₂/N₂ selectivity rose from 1.93 to 6.66 (245%) and CO₂/CH₄ selectivity increased from 6.06 to 33.79 (458%). The enhancements in selectivity were attributed to structural changes in the membrane, which became denser and smoother, as revealed by the SEM images. However, the permeances of all gases dropped with longer heating periods due to the reduced segmental mobility of the polymer, as indicated by DSC analysis. This study explores heating treatment as a method to improve adhesion between the polymer matrix and filler particles.

Keywords: polysulfone-zeolite templated carbon, heating, gas separation, mixed matrix membrane

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HALAL-COMPLIANT ORGANOCLAY FROM PLANT-BASED SURFACTANTS: A GREEN APPROACH FOR FOOD-GRADE MONTMORILLONITE MODIFICATION

**Mohd Aidil Adhha Abdullah^{a,*}, Nur Aliaa Zulkefli^a, Mazidah Mamat^a,
Mohamad Khairi Mohd Zainol^b, Norizah binti Mhd Sarbon^b and Azlin Fazlina bt Osman^c**

^a Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030 Kuala Terengganu, Terengganu.

^a Faculty of Faculty of Fisheries and Food Science, Universiti Malaysia Terengganu, 21030 Kuala Terengganu, Terengganu.

^c Biomedical and Nanotechnology Research Group, Center of Excellent Geopolymer and Green Technology (CEGeoTech), Universiti Malaysia Perlis (UniMAP), Arau 02600, Malaysia

*Corresponding author: aidil@umt.edu.my

Abstract

Sodium montmorillonite (Na-MMT) serves as a popular nanofiller in polymer-based materials; however, its inherent hydrophilicity restricts its interaction with hydrophobic polymer matrices. To improve compatibility, surface treatment with organic surfactants is commonly performed. Traditional methods typically rely on animal-derived surfactants such as hydrogenated tallow, which can be problematic for halal-sensitive applications like food packaging. This study focuses on modifying Na-MMT using plant-based quaternary ammonium compounds—specifically, myristyltrimethylammonium bromide (MTAB) and cetyltrimethylammonium bromide (CTAB)—to promote sustainability and religious compliance. Ion-exchange reactions were used to intercalate these surfactants into Na-MMT at concentrations of 0.5 to 2.0 times the cation exchange capacity (CEC). Structural and morphological changes were examined using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), CHNS elemental analysis, thermogravimetric analysis (TGA) and water contact angle measurements. FTIR spectra verified surfactant inclusion, and XRD revealed expanded basal spacing, more pronounced in samples modified with longer alkyl chains. Thermal behavior, as assessed by TGA, varied depending on surfactant type and loading. Increased hydrophobicity was demonstrated through contact angle testing, especially for CTAB- and MTAB-treated clays. The findings highlight the effectiveness of MTAB and CTAB as plant-derived modifiers, offering a reliable, halal-compliant alternative for enhancing Na-MMT in nanocomposite formulations suitable for food packaging.

Keywords: Halal organoclay, Sustainable surfactants, Food packaging, Montmorillonite modification, Plant-derived surfactants

EXTENDING WOOD LIFESPAN USING GREEN AND ADVANCED CHEMICAL PRESERVATION TECHNOLOGY FOR SUSTAINABLE BUILDING PRACTICES

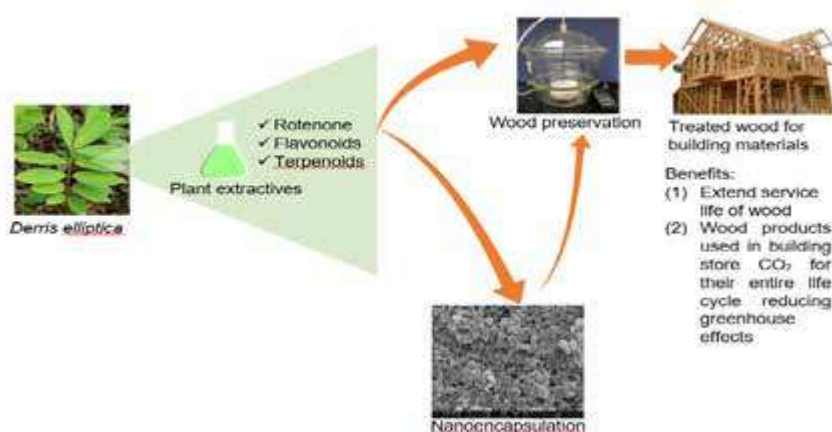
Tumirah Khadiran^{a*}, Mohd Amirul Mukmin Abdullah^a,

^a Wood Protection Branch, Forest Products Division,
Forest Research Institute Malaysia (FRIM), 52109 Kepong, Selangor
*Corresponding author: tumirah@frim.gov.my

Abstract

Wood preservation plays a crucial role in sustainable building practices by extending the lifespan of wood products, reducing the need for frequent replacement, thus minimizing deforestation, which indirectly reduce carbon emission. Additionally, emphasizing wood preservation not only enhances structural durability but also reinforces the principles of sustainability and climate responsibility in the construction industry. We have been studying development of green and advanced chemicals as a wood preservative, which shows a good performance in protecting wood-based products from biodegradation agent attacks likes termites, insects and decay fungi. Herein discussion will be focused on the following points, with the goal of exploring of chemicals that can function to protect wood and prolong its service live: (a) plant extractive as a green chemical to preserve wood^{1,2} and (b) synthesis of nanopreservatives as an advanced wood preservative³. The ability of sound, green, and advanced chemical preservation techniques to extend the lifespan of wood – and their contribution to the achievement of the Sustainable Development Goals (SDGs) – will also be discussed.

Keywords: Wood preservation, nanopreservatives, green chemicals, nanopreservatives, sustainable building practices



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SUSTAINABLE BIOPOLYMER PRODUCTION: TRANSFORMING OIL PALM WASTE INTO PEG-co-FDCA

Mary Hui Yee Ling^a, Joel Hooper^{b,c}, Janarthanan Pushpamalar^{a,d,*}

^a*School of Science, Monash University Malaysia, Jalan Lagoon Selatan, 47500 Bandar Sunway, Selangor, Malaysia.*

^b*School of Chemistry, Monash University, Wellington Road, Clayton VIC 3800, Australia.*

^c*Bioresource Processing Institute of Australia (BioPRIA), Department of Chemical and Biological Engineering, Monash University, Clayton VIC 3800, Australia.*

^d*Monash-Industry Plant Oils Research Laboratory (MIPO), Monash University Malaysia, Jalan Lagoon Selatan, 47500 Bandar Sunway, Selangor, Malaysia.*

*Corresponding author: pushpa.janarthanan@monash.edu; pjanarth72@gmail.com

Abstract

The 2,5-furandicarboxylic acid (FDCA) is a valuable compound in the development of sustainable plastics, primarily serving as a building block for renewable alternatives to aromatic polyesters. Objectives: This study describes the synthesis of FDCA from oil palm empty fruit bunch (OPEFB) and its copolymerization with polyethylene glycol (PEG). Cellulose (53% yield) was extracted then hydrolyzed to glucose enzymatically (62% yield) which was then further dehydrated to 5-hydroxymethylfurfural (HMF) (48% yield) using a safer and greener solvent. The HMF was oxidized to FDCA under mild reaction conditions (67% yield). Then, FDCA was successfully co-polymerized with PEG using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) and N-hydroxysuccinimide (NHS) coupling mechanism to form PEG-co-FDCA with 58% yield. The PEG-co-FDCA was found to be semicrystalline structure (50% crystallinity) and showed crystalline lamellae and amorphous clusters. This was verified with the VPSEM images that showed crystalline lamellae and amorphous clusters. The measurements of molecular weight and particle size ($15,400 \pm 200$ g/mol; 369.97 nm) indicated the formation of a larger polymeric chain. Finally, T_m , T_g , and T_{d-max} was determined to be 67.33, 26.76, and 468.53 °C respectively via DSC and TGA. The use of OPEFB in the production of PEG-co-FDCA offers a sustainable solution to waste management and environmental challenges. The resulting PEG-co-FDCA can be used to produce bioplastics, coatings, adhesives, and biodegradable fibers for the textile industry, providing a sustainable alternative to conventional plastics adhering to the UN Sustainable Development Goal. This shift towards renewable resources like OPEFB decreases dependency on fossil fuels, further reduces carbon emissions and promotes a circular economy addressing the UN Sustainable Development Goal of Responsible Consumption and Production (SDG12), Climate Action (SDG13), Life on Land (SDG15).

Keywords: FDCA, biodegradable plastic, PEG, copolymerization, oil palm empty fruit bunch

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GREEN TECHNOLOGY APPROACH FOR SYNTHESIZING THERMOPLASTIC ROAD MARKING PAINT USING SUSTAINABLE BIOMASS FOR CARBON DIOXIDE REDUCTION

Wan Nur Aqlima Wan Ali^{a,*}, Rozzeta Dolah^a, Sheikh Ahmad Zaki^b, Siti NorHuda Abdullah^c,

^a*Faculty of Artificial Intelligence, Universiti Teknologi Malaysia, 54100 Kuala Lumpur, Malaysia.*

^b*Malaysian-Japan International Institute of Technology, Universiti Teknologi Malaysia, 54100 Kuala Lumpur, Malaysia*

^c*Faculty of Civil Engineering, Univerisiti Teknologi Malaysia, 81310, Johor, Malaysia*

**Corresponding author: wannuraqlimawanali@graduate.utm.my*

Abstract

Thermoplastic road marking paint have been used to enhance safety features in road and building. Traditional thermoplastic paints, widely used for road marking, often rely on petroleum-based components, contributing to significant greenhouse gas emissions. This study explores the enhancement and application of thermoplastic road marking paint by incorporating sustainable materials such as lignin, cellulose fibers, and renewable resins. The primary objective is to investigate the potential of incorporating sustainable materials into thermoplastic road marking paint formulations to reduce carbon dioxide emissions while maintaining high performance and durability. Besides that, this research evaluated the mechanical properties, environmental impact, and longevity of the enhanced road marking paint through testing. Mechanical testing is conducted to evaluate properties such as reflectivity (R_L) of the thermoplastic road marking paint. The results indicate that the sustainable formulation improves the mechanical performance of the thermoplastic road marking paint, achieving an RL value of 417 mcd/m²/lx compared to the standard RL of 336 mcd/m²/lx. Furthermore, the thermoplastic road marking paint was synthesized and characterized using X-ray diffraction (XRD) analysis to determine the crystalline structure and phase composition for carbon dioxide adsorption. This innovative approach presents a promising pathway for the transportation industry to align with sustainability goals while ensuring road safety and functionality.

Keywords: Thermoplastic Road marking, carbon dioxide adsorption, reflectivity, sustainable material

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INTEGRATED REAL-TIME ENVIRONMENTAL MONITORING AND MORPHOLOGICAL CHARACTERIZATION OF NANO-CARBON PAINT FOR CARBON EMISSION REDUCTION IN GREEN TECHNOLOGY APPLICATIONS

Siti Norhuda Abdullah^{a,*}, Rozzeta Dolah^b, Shazwin Mat Taib^a, Wan Nur Aqlima Wan Ali^b,
Mohamad Afiq Roslan^c

^aFaculty of Civil Engineering, Universiti Teknologi Malaysia, 81310, Skudai, Johor, Malaysia.

^bFaculty of Artificial Intelligence, Universiti Teknologi Malaysia, 54100, Kuala Lumpur, Malaysia.

^cNaglus Industries Sdn. Bhd., i-13, i-Cube Incubator, Block J3, Level 2, Universiti Teknologi Malaysia, 54100, Kuala Lumpur, Malaysia.

*Corresponding author: sitinorhuda@graduate.utm.my

Abstract

In response to the urgent need for carbon emission reduction, this study explores the potential of nano-carbon paint as a sustainable coating material for green technology applications. The research integrates real-time environmental monitoring with comprehensive morphological and structural analyses to evaluate the carbon adsorption performance of nano-carbon paint in comparison to a conventional commercial Brand X paint. Two identical house prototypes were constructed under controlled tropical conditions: one coated with a laboratory-formulated nano-carbon paint and the other with Brand X. A dual-method approach was employed; (1) on-site monitoring of ambient carbon concentrations over a 24 hours period using non-dispersive infrared (NDIR) CO₂ sensors, and (2) laboratory-based analysis of the paint's structural and chemical characteristics. Scanning Electron Microscopy (SEM) revealed that the nano-carbon paint exhibited a highly porous and flaky surface morphology, enhancing surface area and promoting carbon interaction. X-ray Diffraction (XRD) analysis confirmed the presence of ordered graphitic structures, while Fourier-Transform Infrared Spectroscopy (FTIR) identified functional groups indicative of active carbon bonding sites, supporting its carbon adsorption capabilities. Real-time environmental data showed that the nano-carbon-coated prototype achieved a 28% reduction in ambient carbon levels compared to the Brand X-coated control, with a mean concentration difference of 136 ppm. This demonstrates the superior passive carbon mitigation performance of the nano-carbon formulation. This study underscores the potential of functional nano-coatings in promoting low-emission architecture and supports their further development and application in sustainable building practices.

Keywords: Nano-carbon paint, biomass waste, carbon reduction, nanotechnology, green building technology

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SYNTHESIS OF NICKEL COBALT ELECTROCATALYST VIA FACILE HYDROTHERMAL METHOD FOR HYDROGEN EVOLUTION REACTION

Nurulfasihah Azhar^a, Rozan Mohamad Yunus^{a,*} Azim Fitri Zainul Abidin^a,
Rabiatul Adawiyah Mohd Shah^a, Ng Wei Shi^a

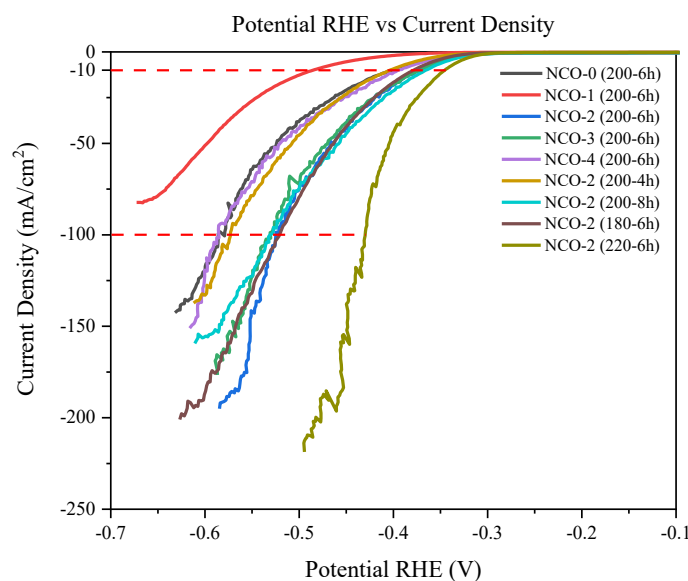
^aFuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia.

*Corresponding author: rozanyunus@ukm.edu.my

Abstract

Ni-based electrocatalysts have emerged as cost-effective and high-performance alternatives to noble-metal catalysts for the hydrogen evolution reaction (HER)¹. However, pure Ni electrocatalysts exhibit relatively high overpotentials due to their strong hydrogen adsorption energy, which limits the efficiency of hydrogen desorption and results in sluggish HER kinetics. To address this, alloying nickel (Ni) with other transition metals like cobalt (Co) leverages synergistic effects in the electronic structure, producing highly active and durable HER electrocatalysts^{2,3}. In this study, we employed a hydrothermal approach to synthesize NiCo₂O₄, followed by an annealing process to reduce NiCo₂O₄ into NiCo alloy. Given the versatility of the hydrothermal method for synthesizing NiCo electrocatalysts, we studied how hydrothermal duration and temperature affect NiCo growth and electrocatalytic activity⁴. Our results indicate that both hydrothermal duration and temperature significantly affect the morphology of NiCo, which in turn influences its catalytic performance. Finally, we discuss possible improvements in hydrothermal synthesis that could further enhance electrocatalytic activity.

Keywords: electrocatalysts, transition metals, hydrogen evolution reaction, hydrothermal method, electrocatalytic activity



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THE ETHICAL DIMENSION OF GREEN CHEMISTRY: PATHWAYS TO A SUSTAINABLE FUTURE

Mani Omprakash Srivastava

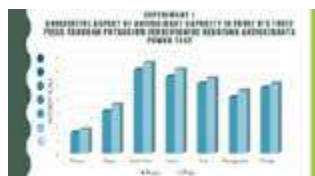
*School Principal and Chemistry educator
New Horizon Scholars School, Mumbai, India
Corresponding author: manellin@yahoo.com

Abstract

An amalgamation of GREEN CHEMISTRY and ethical education to prepare learners and spread the green culture with an army of green tender hearts to conserve Mother Earth and respect Nature's serenity, tranquility and magnificence. Ethical and green sustainability pledge with joint research projects is to prepare the subsequent generation of learners for persuading and propagating principled and responsible revolutions which will empower learners and will result in no more disastrous constituents in substance of a viable Planet. A novel approach towards GREEN Chemistry education and Moral Code in Chemistry Education is TO CREATE ETHICAL IDEOLOGY. Shifting the Paradigm by embracing an interdisciplinary approach of ethical imagination and invention. Designed and implemented different researches towards a greener prospective program with full involvement of students, teachers and local communities. It's to Initiate and prepare the subsequent generation of chemists and scientist by empowering them towards a fundamental change in society by bringing a radical revolution in human mind to develop an understanding that Chemistry is to CREATE NOT DESTROY. Developed a zero-tolerance approach towards ignorance and negligence in scientific inventions by highlighting the understanding towards whose responsibility is deadly plastics which has become threatening to all life, CFC generated broad spectrum thinning of ozone layers, heavy metal hazards, oil spill, COVID-19... many like these represents a big concern towards our planet and makes big inventions in vain. Inducing every learner and teachers towards the protection of environment and to protect humanity on Planet earth. The students were instilled with the oft repeated thought that, 'We have not inherited this earth from our forefathers; we have borrowed it from our children'. Bridging the gap between green chemistry and sustainable education through ethical green expansions is by connecting the dots across as individuals, society, community, country and world. Through an approach that provides a framework to integrate sustainability principles and grow their minds to innovate and become curator of our Universe, with their skill to protect our planet's peace, calmness and radiance for future generations. Ethical Imagination and invention transform the way of education is experienced inspiring young people to discover that there is far more within them than they think, to discover their grand passion in life and to explore what it means to live from a strong sense of responsibility.

Keywords: sustainable world, green curriculum, green pledge, ignorance inventions

Undertook various projects covering a wide expanse of soil and water, wherein the stress was not on the staple move of removing the irritants but to utilize them in a better manner so as to fulfill our dreams of a Healthy and Green World. Working on this line, we tried to use the industrial waste, discarded objects and contaminated water in an exhaustive manner to get rid of their evils and utilize them in a better way for sustainable development. The major Projects are as following:



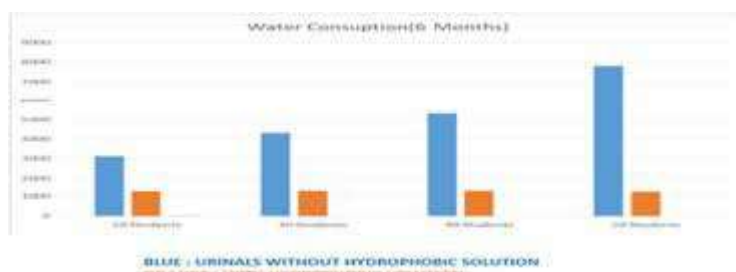
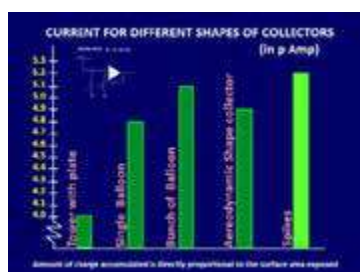
- **Free Radical scavenging activity** by investigating Tagetes Erecta a scavenger of Sullage
- **Nutrameal:** Peel of fruits Antioxidants a hero component terminates the free radical chain reactions before the cell components are destroyed!
- **Removal of Heavy Toxic Metal from waste water:** To make potable water (devoid of Toxic Effluents) and make it available for masses.
- **Designed hydrophobic solution to Solve the Water Crisis:** PMMA and SiO₂ coating Used in Urinal to use water in flushing. A Nano solution to a Giga Nano problem which can save gallons of Water.

~ continue next page ~



- **ATMO POWER:** Design a sustainable world with consideration to environmental impact by harnessing electricity from atmosphere.
- Developed Nutrameal A planetary Health diet to Save Earth before its too late and also for lower starta people: Nutrameal from weeds a cost-effective food supplement to combat dietary deficiencies and malnutrition as it provides balance diet in single food.
- Bio Fuel: To create most valuable form of renewable energy a transportation fuel options to establish safe, clean and sustainable hydrocarbon.
- Offsetting Carbon Emission with Emerging Technologies; To reduce dependency on hydrocarbon for fueling the transportation and other sector; to provide more economic opportunities for the development of the country' to reduce carbon foot print and save our environment for the future generation.

In an ideal world, Education for GREEN Viable Advancement should pervade the entire school curriculum, with every subject area, at every year level, dealing with aspects of sustainability in broader way.



Reference and acknowledgement

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5. Agriculture university Pune, Maharashtra
6. Subodh laboratories, Turbhe Maharashtra
7. Infinity lab solutions, Nerul, Maharashtra
8. Maharashtra pollution control department.
9. Bokarpada water purification Centre
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SYNTHESIS OF SORBENTS FOR CO₂ CAPTURE FROM CONSTRUCTION AND DEMOLITION WASTE AS RAW MATERIALS

Yergaziyeva G.Y.^{1,2*}, Myltykbayeva L.K.¹, Makayeva N.M.^{1, 2}, Mambetova M.M.^{1,2},
Dossumov K.¹, Anissova M.M.¹.

¹Center of Physical Chemical Methods of Research and Analysis, Al-Farabi Kazakh National University, Tole Bi str. 96A, Almaty 050012, Kazakhstan

²The Laboratory of Catalytic Processes, Institute of Combustion Problems, Bogenbay Batyr Str. 172, Almaty 050012, Kazakhstan

*Corresponding author: ergazieva_g@mail.ru

Abstract

One of the major problems facing humanity that affects economic, social and environmental aspects is climate change. The main cause of climate change is the increase in greenhouse gases, particularly carbon dioxide (CO₂), which is the largest contributor to the greenhouse effect. Kazakhstan ranks 10th in the world in greenhouse gas emissions per capita with 18 tons of CO₂ per year, highlighting the importance of addressing the issue of CO₂ utilization at both the international and national levels.

Promising methods to reduce CO₂ emissions include CO₂ capture and utilization from exhaust gases. Bifunctional materials based on lithium silicates obtained from construction waste show great potential due to their low cost and environmental benefits. Construction waste in Kazakhstan is mainly disposed of in landfills, making their reuse as a source of silicon for lithium silicates a promising approach. These silicates have high thermal and chemical stability, making them effective for CO₂ capture and utilization, although further research is needed to optimize production and industrial application. Lithium silicates were synthesized using self-propagating high-temperature synthesis (SHS), alkali fusion and mixing methods from silicon-rich construction waste such as sand and clay. Elemental analysis showed that clay and sand had the highest silica content (72.2% and 68.3%, respectively), making them most suitable for lithium silicate synthesis. Samples prepared by the SHS method contained only 4–5% lithium orthosilicate (Li₄SiO₄), highlighting the need for synthesis optimization. In the alkali fusion method, increasing the Li:Si ratio from 1.5:1 to 4:1 increased the Li₄SiO₄ content from 44% to 90%. In contrast, in the mixing method, the Li₄SiO₄ content peaked at 93% at a ratio of 1.5:1 but decreased at higher ratios. These results highlight the critical role of Li:Si ratio and synthesis conditions in achieving high-quality lithium silicates for efficient CO₂ capture.

Keywords: sorbent, CO₂ capture, lithium silicates, waste

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ENHANCING GENERAL CHEMISTRY EDUCATION FOR ALLIED HEALTH: DEVELOPMENT AND VALIDATION OF GREENLAB, A GREEN CHEMISTRY- INTENSIVE LABORATORY MANUAL

Romulo R. Macadangdang Jr.^{a,*}

^a*National University, Philippines, 551MF Jhocson St., Sampaloc, Manila, Philippines*

^{*}*Corresponding author: rjrrmacadangdang@national-u.edu.ph*

Abstract

This study presents the development and validation of the GreenLab Laboratory Manual, a green chemistry-intensive instructional tool tailored for general chemistry courses in allied health programs. GreenLab addresses an educational gap in sustainability within healthcare fields by integrating principles such as waste prevention, safer solvents, renewable feed stocks, and resource-efficient practices into laboratory activities. Using the ADDIE instructional design model—Analysis, Design, Development, Implementation, and Evaluation—the manual was systematically crafted to meet the educational requirements of allied health students, aligning laboratory practices with global environmental standards and the United Nations Sustainable Development Goals.

Employing experimental research design, this study involved control and experimental groups from comparable allied health courses. Students in the experimental group used the GreenLab Manual over a six-week period, while the control group engaged in traditional laboratory exercises. Pre-test and post-test assessments were administered to evaluate the students' understanding of green chemistry principles. The results revealed a marked improvement in the experimental group, with students demonstrating a “very high level of understanding” of green chemistry concepts, while the control group showed only modest gains. Qualitative feedback further indicated that the manual fostered heightened environmental awareness and encouraged critical thinking, although some students suggested enhancements like glossaries and visual aids for improved comprehension.

The study confirms the GreenLab Manual's effectiveness in advancing allied health students' knowledge of sustainable chemistry. By bridging academic content with practical applications, GreenLab offers a replicable model for integrating green chemistry principles into science education, equipping future healthcare professionals with the knowledge to practice environmentally responsible chemistry. This work contributes valuable insights toward sustainable education in healthcare, supporting a broader movement for ecological stewardship.

Keywords: Green chemistry, allied health education, sustainable chemistry, instructional design, environmental awareness

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TOWARDS SUSTAINABLE PLANTATION STRATEGIES VIA APPLICATION OF NANOFERTILIZERS FOR NUTRIENT EFFICIENCY

Nor Farhana Khadiran^{a,*}, V. Jeyanny Vijayanathan^a, Rosdi Koter^a, Rozita Ahmad^a, Izwan Jaimi^a,
Amir Nordin^a, Salwana Hashim^a,

^aSoil Management Branch, Forest Plantation Programme, Forest Biotechnology Division,
Forest Research Institute Malaysia, 52109 Kepong, Selangor.

*Corresponding author: norfarhana@frim.gov.my

Abstract

The increasing demand for sustainable agriculture has driven the development of innovative nanofertilizers to enhance nutrient limitations, particularly zinc and nitrogen deficiencies. Nanofertilizers such as Zinc Layered Hydroxide Nitrate (ZLH-NO₃⁻) with their nanoscale particle size and high surface area offer a novel approach in a sustainable solution by slow-release mechanism. nanofertilizer ensures a steady supply of essential nutrients, reducing nutrient losses through leaching and volatilization, thereby improving plant uptake efficiency (Liu & Lal, 2021) and minimizing environmental pollution (Mahajan , Dhoke, & Khanna, 2022). Besides, this innovation plays a crucial role in smart agriculture by optimizing resource use, reducing dependency on chemical fertilizers, and mitigating climate change through lower carbon footprints (Raliya , Saharan V, Dimkpa, & Biswas , 2018). This investigation was done to determine the release of nano-fertilizer and nutrient uptake by Kelampayan seedlings (*Neolamarckia cadamba*). The plant tissue samples were collected from Kelampayan seedlings (*Neolamarckia cadamba*) after 4 months after Nano-Fertilizer application and processed to undergo nutrients analysis using ICP-OES instrument and CNS analyzer. Results revealed that the biomass wet weight obtained from treatments with Nano-Fertilizer application reached to 33.6 g significantly different compared to commercial fertilizer (20.3g). This could be related to the slow release properties of Nano-Fertilizer, which improved the nutrient release and increased the biomass yield. Besides, the concentration of N, P and Zn in Kelampayan leaf (*Neolamarckia cadamba*) from treatment using Nano-Fertilizer application gave the highest values of 2.14%, 0.22% and 96.8 ppm, respectively compared to commercial fertilizer (1.55%, 0.19% and 55.9 ppm) accordingly. This trend was consistent with the highest biomass weight observed in the same treatment. This supported the idea that slow release properties of nano-fertilizer can improve nutrient uptake in plants and enhance the growth performance of Kelempayan with an increase in biomass yield, Application of nano-fertilizer also reduces excessive fertilizer application, thereby providing a strategy to mitigate excessive greenhouse gas emissions and environmental degradation.

Keywords: nano-fertilizer, zinc layered hydroxide nitrate, nutrient efficiency, smart agriculture, climate change mitigation

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ONE POT SYNTHESIS OF 3,4-DIHYDRO-3-HYDROXYISOCHROMAN-1-ONE AND EVALUATION OF ITS ACETAL DERIVATIVES AS NEW CLASS OF MOSQUITOCIDAL COMPOUNDS

Gautam M. Patel^a and Pradeep T. Deota^b

^a*Chemistry Department, Parul Institute of Applied Science, Parul University, Vadodara-391760, Gujarat, India.*

^b*Applied Chemistry Department, Faculty of Technology & Engineering,
The Maharaja Sayajirao University of Baroda, Vadodara, India.*

**Corresponding author: gautampatel1573@yahoo.co.in*

Abstract

First one-pot synthesis of 3,4-dihydro-3-hydroxyisochroman-1-one (lactol) from indene using tungstic acid-hydrogen peroxide is reported and a plausible mechanism of its formation is also proposed by different experimental studies. The synthesized lactol was further converted into its novel acetal derivatives. All the synthesized compounds were evaluated for their mosquitocidal activity on mosquito species, *Anopheles Culicifacies* using standard WHO specified adult susceptibility test. The results revealed that all the compounds encompassed excellent mosquitocidal activity. Further all the compounds are tested for cytotoxicity on human lung cell line L132. The results of the studies exhibited lactol are less toxic to human body than existing mosquitocidal compounds.

Keywords: lactol, acetals, *anopheles culicifacies*, mosquitocidal.

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DRIVING CHEMISTRY FOR SUSTAINABLE CHANGE

Mandar Bodas*

¹ Elsevier India; ² Elsevier Taiwan; ³ Elsevier Singapore

*mandar.bodas@elsevier.com

Abstract

Modern chemistry is the backbone of our society and has a profound impact on our lives. The chemical sector consumes 10% of the world's total energy and contributes to 8% of greenhouse gas emissions. 90% of global production depends on chemical products. Chemistry also is a major contributor to global environmental pollution, plastic waste and the ongoing climate crisis based on the products we use such as detergents, toothpaste, plastic, paints, drugs and beyond. The transition toward a sustainable future is the key for radical transformation towards sustainability to meet these global challenges on how chemistry is designed, developed, and executed. Sustainability-focused chemistry research is key to realizing lower pollution levels, less waste, safer chemicals, and greater energy efficiency. To adapt to a changing world, chemical syntheses and processes need to be adapted too.

Sustainable Chemistry makes a critical contribution to achieving the aims of all SDGs. Reaxys database along with the interoperability experience from ScienceDirect and Scopus database helps researchers in providing the right solutions which saves time and cost by improving efficiency and productivity.

Reaxys retrieves literature, compound properties and chemical reaction data faster than any other solution Reaxys offers a highly intuitive interface and robust database to help leading chemists retrieve relevant chemical literature, patent information, valid compound properties and experimental procedures in half the time. Designed to support the full range of chemistry research, including pharmaceutical development, environmental health & safety work and material science, Reaxys puts every scientist, from novice to expert, on the shortest path to answers.

Keywords: Green chemistry; sustainable chemistry; Reaxys; synthesis; chemistry research.

INNOVATING GREEN AND LOW-CARBON TECHNOLOGIES TO ENABLE CARBON PEAKING AND CARBON NEUTRALITY: PROGRESS OF GREEN CARBON

Xiang Qiu^{a*}

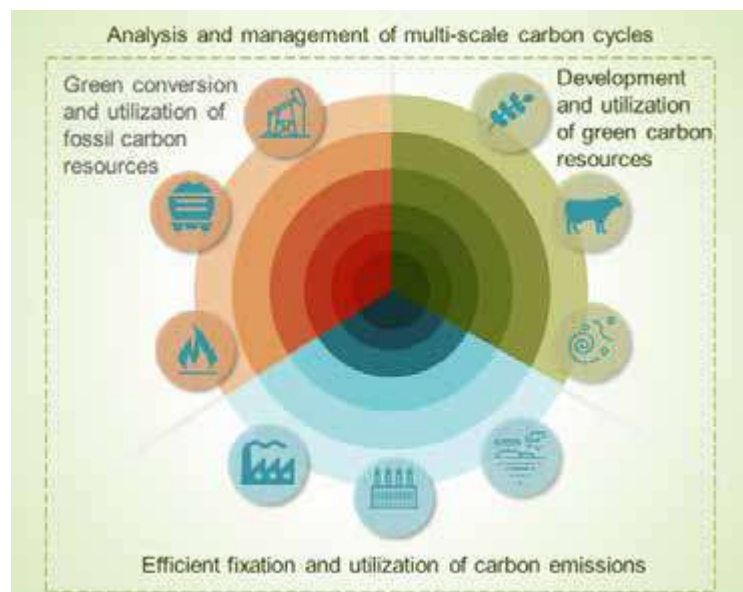
^aGreen Carbon Journal Center, Qingdao Institute of Bioenergy and Bioprocess Technology,
Chinese Academy of Sciences, Qingdao, China

* Corresponding author: qiuxiang@qibebt.ac.cn

Abstract

Green Carbon (ISSN 2950-1555) is an open-access English academic journal founded by the Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, in response to United Nations Sustainable Development Goal 13 (Climate Action). It is an interdisciplinary journal dedicated to promoting cutting-edge scientific and technological developments in green resources, green conversions, green processes, and green products that lead to low, zero, or negative carbon emissions. Green Carbon strives to be among the top 10% of journals in the field of low-carbon sustainable development technology. The presentation will provide a comprehensive overview of the journal's progress since its inception, detailing its organizational structure, article publication, promotional activities, and publicity efforts.

Keywords: Green Carbon, interdisciplinary journal, low-carbon sustainable development





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and 50th World Chemistry Congress (50WCC)**

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ADVANCED INTELLIGENT SYNTHESIS PLATFORM EMPOWERED BY HIGH-PRECISION INSTRUMENTATION

Xuefeng Jiang^{1*}

¹*School of Chemistry and Molecular Engineering, East China Normal University, Shanghai 200062, China*

**Corresponding author: xfjiang@chem.ecnu.edu.cn*

Abstract

The rapid development of artificial intelligence (AI) is ushering in a paradigm shift in chemistry. Digital chemistry, which integrates automated equipment, machine learning algorithms, and big data applications, bridges digital technologies with practical chemistry to accelerate the discovery of new compound.^[1] We have overcome key bottlenecks in photo- and electro- sciences, particularly in scale-process, addressing challenges in photocatalyst recovery, multiphase catalysis, and heterogeneous photocatalyst immobilization. 1) Based on the Beer-Lambert law, the inverse square law, and Lambert's cosine law, the synergistic relationship between reaction systems and light sources has been established.^[2] Fundamental principles for photoreactor have been proposed, emphasizing stability, reproducibility, parameter adjustability, precise thermal and mass transfer, and accurate functional integration.^[3] 2) Through advancements in constant-pressure and constant-current switching, we have resolved electrode surface deposition effects via program-controlled phase-shift alternating current, enabling the introduction of diverse waveforms for current and voltage. These advancements in the standardization and precision of synthetic instruments have transformed data into massive and precise, driving automation and intelligent synthesis in synthetic chemistry, materials science, and drug discovery.^[4]



Keywords: high-precision instruments, intelligent platforms, photo/electro-catalysis, big data.

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QUANTUM MACHINE LEARNING FOR MOLECULES – A HYBRID QUANTUM NEURAL WAVEFUNCTION APPROACH

Weitang Li, Zhigang Shuai

School of Science and Engineering,

The Chinese University of Hong Kong, Shenzhen, 518172 Guangdong, People's Republic of China

**Corresponding author: shuaizhigang@cuhk.edu.cn*

Abstract

We introduce a hybrid framework to describe molecular wavefunction using a combination of an efficient quantum circuit and a neural network. Numerical benchmarking on molecular systems shows that our hybrid quantum-neural wavefunction approach achieves near-chemical accuracy, comparable to advanced quantum and classical techniques. Taking the isomerization reaction of cyclobutadiene as an example, which has been considered as a challenging issue with multireference feature or strong correlation effect, our approach is validated on a superconducting quantum computer with high accuracy and significant resilience to noise.

INTEGRATION OF AI TOOLS INTO CHEMISTRY RESEARCH

Valentine P. Ananikov

Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences

Leninsky prospekt 47, Moscow; <http://AnanikovLab.ru>

**Corresponding author: val@ioc.ac.ru*

Abstract

The rapid advancement of artificial intelligence (AI) technologies is reshaping the landscape of chemistry research, providing transformative tools for addressing long-standing challenges in data interpretation, molecular design, and reaction discovery. Integrating AI into the chemical sciences involves not only applying algorithms to large datasets but also rethinking the nature of chemical knowledge itself. Recent studies have demonstrated the power of machine learning and neural networks to uncover hidden patterns in reaction mechanisms, explore the dynamic behavior of catalytic systems, and predict synthetic outcomes with remarkable accuracy. AI-based analysis of structural and reactivity data enables the revival and systematization of overlooked chemical information, as shown in the reconstruction of “sleeping” knowledge from experimental reports and literature. Moreover, intelligent digital assistants can help navigate complex reaction networks, guiding chemists through multidimensional parameter spaces toward optimized conditions and novel synthetic pathways. These developments reflect a broader trend toward the digitization of chemical knowledge, where AI serves as a bridge between raw experimental data and conceptual understanding. Successful integration of AI requires careful attention to data quality, domain-specific representation, and collaboration between chemists and data scientists. As we move toward a more interconnected and knowledge-driven discipline, AI is expected to become an integral component of modern chemical research, enhancing creativity, precision, and reproducibility. Our recent results [15] along with current leading trends in AI-driven chemical research will be presented and discussed.

Keywords: artificial intelligence, chemical data, catalysis, machine learning, reaction networks.

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AI FOR LEARNING ACROSS CHEMICAL SPACE AND QUANTUM CHEMICAL METHODS

Pavlo O. Dral^{a,b,*}

^aPCOSS, FTCC, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

^bInstitute of Physics, Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University in Toruń, ul. Grudziądzka 5, 87-100 Toruń, Poland

*Corresponding author: dral@xmu.edu.cn

Abstract

Our work focuses on using AI to accelerate and improve the accuracy of molecular simulations at the quantum chemical level. We developed a range of methods, most of which can make predictions faster and more accurately than popular DFT approaches such as B3LYP/6-31G* without needing to be trained, i.e., they can be directly used as DFT approaches across the chemical space. The first successful example of such an approach is the AIQM1 method¹ approaching CCSD(T)/CBS accuracy at the semi-empirical cost. AIQM1 was proven efficient for simulations ranging from accurate ground-state geometry optimizations, thermochemical calculations, and dynamics to excited-state property predictions. We have developed a series of the successors of AIQM1 collected in the universal and updatable AI-enhanced quantum mechanical (UAIQM) models.² These models mark the paradigm change in computational chemistry towards auto-selection of the best approach for the given time budget with the capability to be continuously improved with more usage. We also introduced many more novel approaches for learning across different quantum chemical levels, e.g., DFT ensembles³ and all-in-one models⁴. Our methods are available in the MLatom⁵ package for AI-enhanced computational chemistry.

Keywords: AI, ML, quantum chemistry

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ARTIFICIAL NEURAL NETWORKS FOR THE ANALYSIS OF MICROSCOPY DATA

Nartova A.V.^{a,b*}, Matveev A.V.^b, Okunev A.G.^b

^a*Boreskov Institute of Catalysis SB RAS, 630090 (Russia)*

^b*Novosibirsk State University, 630090 (Russia)*

*Corresponding author: nartova@catalysis.ru

Abstract

The search for different types of objects and determine the parameters in different types of images is the one of the common tasks in various fields of science and technology. Objects, such as particles, quantum dots, crystals, defects, pores, cells, bubbles, etc., can be of different sizes and shapes. The parameters of interest for objects can be the number of objects, their size, area, degree of elongation, concentration, coverage, etc. To obtain relevant statistical data, it is necessary to count and measure hundreds of objects under study, the more the better. This routine work is time consuming. Thus, finding a way to automatically process images to obtain an adequate result is a very important task for modern technologies. An approach to automating image analysis based on deep machine learning is presented [1-4]. It is demonstrated how a neural network (NN) can be used to recognize objects in images of different types and provide information for statistical analysis. The advantages and limitations of the approaches are discussed. A universal, user-friendly online platform iOk (<https://iok.nsu.ru/>) is described. The platform combines the ParticlesNN web service (<http://particlesnn.nsu.ru/>) and the DLgram (https://t.me/nanoparticles_nsk) and No Code ML (https://t.me/nsu_ml_bot) cloud services for automatic recognition of any type of object in images of any quality. The usage of these services in research work significantly reduces the time spent on quantitative analysis of images, reduces the influence of subjective factors and improves the accuracy of analysis due to a sharp increase in data. Developed the DLgram and No Code ML services allow users to train a NN on their images, makes it universal and suitable for solving a large number of routine tasks. It can be confidently stated that the use of NNs is the most advanced approach to automating the process of microscopic imaging.

Keywords: image microscopy analysis, automatic recognition, deep machine learning, computer vision, neural network

Acknowledgements: This work was supported by the Ministry of Science and Higher Education of the Russian Federation within the governmental order for Boreskov Institute of Catalysis (project FWUR-2024-0032) and by the strategic academic leadership program “Priority 2030” at the Novosibirsk State University.

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APPLICATION OF MACHINE LEARNING TO MASS SPECTROMETRY ANALYSIS OF CATALYTIC SYSTEMS

Julia Burykina^{a,*}, Daniil Boiko^a, Konstantin Kozlov^a, Valentina Ilyushenkova^a.

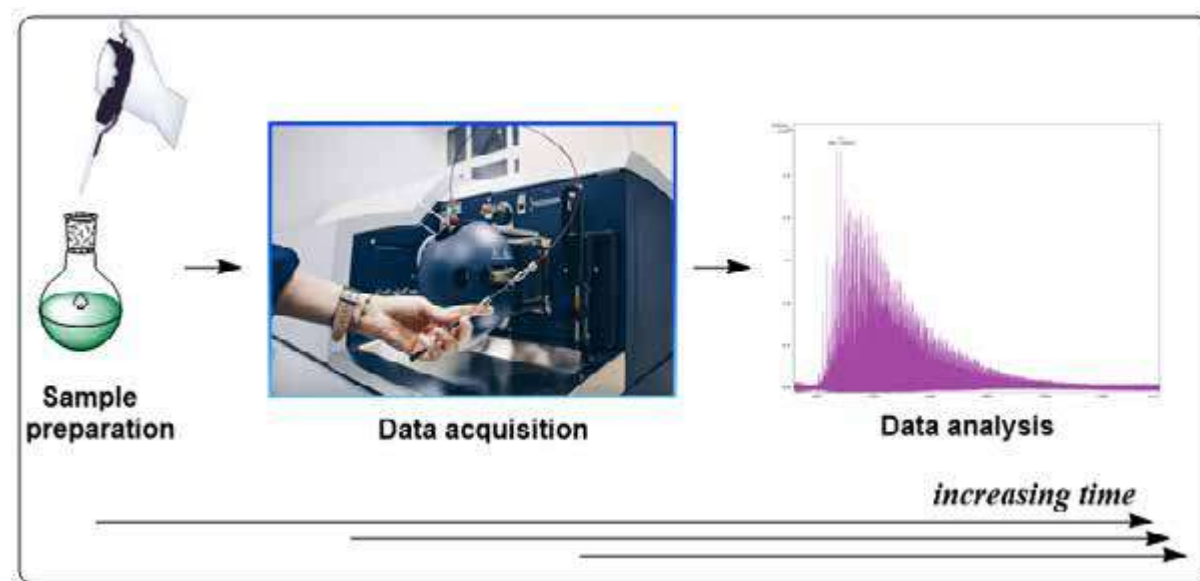
^a *Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences*

**Corresponding author: ivanova@ioc.ac.ru*

Abstract

Mass spectrometry is one of the powerful technique for analyzing a variety types of samples originated from different fields, i.e. petroleomics, metabolomics, proteomics, catalysis, organic synthesis etc.^{1,2} the reaction conditions vary considerably between compound classes, necessitating renewed case-by-case optimization of the reaction conditions⁴. Here we introduce adaptive dynamic homogeneous catalysis (AD-HoC One of the main features of mass spectrometric methods is the comprehensive level of sample characterization and the large amount of data generated, because all compounds that are ionized have their own mass spectral response. The study of organic reactions by mass spectrometry approaches was possible thanks to a grant from the RSF 24-13-00099. It is quite easy to collect a large data set, while the possibilities of manual human analysis are already exceeded.³ Due to this large amount of data is not interpreted and remains unanalyzed. Machine learning techniques can come to the solution, which can fully utilize this data, allowing previously impossible discoveries to be made.⁴

Keywords: electrospray ionization mass spectrometry, machine learning, organic chemistry



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COMPUTER-AIDED ANALYSIS OF LIQUID DYNAMICS CAPTURED BY ELECTRON MICROSCOPY

Alexey S. Kashin^{a,*}

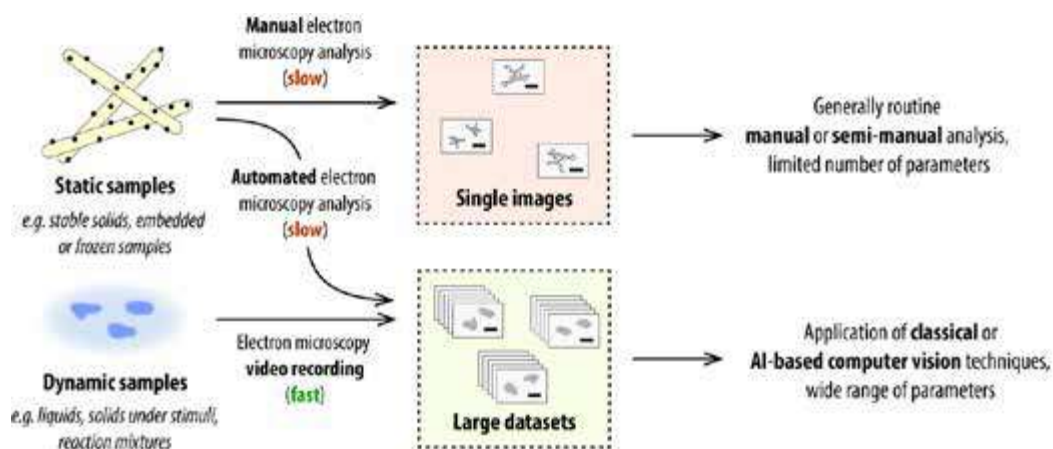
^a*N.D. Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia.*

^{*}*Corresponding author: a.kashin@ioc.ac.ru*

Abstract

Today, almost a century after its introduction, electron microscopy has become an important tool for structural studies in chemistry, materials science and life sciences. The progress made in recent decades in this field has been linked to the ability to study liquid samples under native conditions, which has made electron microscopy a tool for the direct observation of chemical processes in the liquid phase and wet biological systems.¹ An additional advantage of studying liquid samples with electron microscopy is their high mobility, which makes it possible to generate large data sets of images in single experiments in the form of videos that reflect the dynamics of the sample under electron microscope chamber conditions. Fast and qualitative multi-parametric analysis of large amounts of acquired data requires the use of computational image processing methods. Here we present the application of machine learning based methods to study and describe the dynamic behaviour of liquid phase systems based on ionic liquids under scanning electron microscopy observation conditions.^{2,3} Ionic liquids are a unique class of liquid organic salts that tend to form an evolved and mobile microstructure in the liquid phase. This feature of ionic liquids is not only interesting for independent study, but also provides a basis for controlling chemical reactivity in such media.^{4,5} This work was supported by the Russian Science Foundation, RSF grant no. 24-73-10177.

Keywords: microscopy image analysis, computer vision techniques, scanning electron microscopy, liquid dynamics, ionic liquids



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AUTOMATED MACHINE LEARNING WORKFLOWS AND THEIR APPLICATIONS TO LOW-DATA CHEMICAL PROBLEMS

Juan V. Alegre-Requena^{a,*}, David Dalmau,

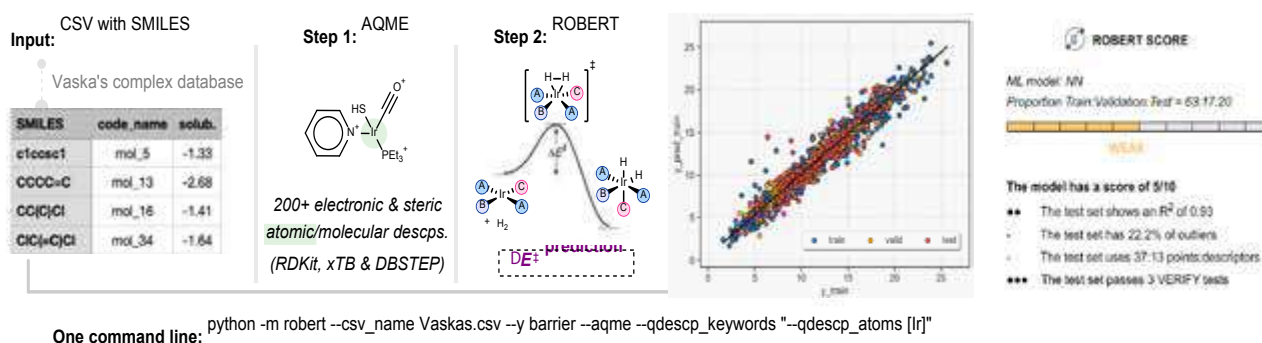
^a Department of Inorganic Chemistry, Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), CSIC-Universidad de Zaragoza. C/ Pedro Cerbuna 12, 50009 Zaragoza (Spain).

*Corresponding author: jv.alegre@csic.es

Abstract

Continued improvements in computer hardware and algorithms have allowed quantum chemical methods to be employed for studying more complex and larger chemical systems. However, performing the various computational protocols required for high-throughput screening, molecular optimization, and machine learning (ML) model training can be tedious and time-consuming. Automating these workflows minimizes errors, enhances reproducibility, and facilitates storing and reusing the associated data. In this work, we present AQME,¹ an automated end-to-end workflow software that performs multi-step tasks of computational chemistry, and ROBERT,² a program that automates ML-related tasks such as data curation, hyperparameter optimization, and ML predictor generation. The combination of these programs allows for high-quality ML predictions to be generated with just one command line or through a graphical user interface, starting from simple inputs such as SMILES strings. We also show how these automated workflows can be useful to study low-data chemical problems containing between 20 and 50 data points.

Keywords: machine learning, automation, workflows, cheminformatics, data-driven



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DATA-EFFICIENT MACHINE LEARNING MODELS FOR TRANSITION METAL SYSTEMS: FROM ^{195}Pt NMR CHEMICAL SHIFTS TO NANOPARTICLE REACTIVITY

Mikhail V. Polynski^{a,*}

^a National University of Singapore, 4 Engineering Drive 4, Singapore 117585, Singapore.

*Corresponding author: polynskimikhail@gmail.com, mvp@nus.edu.sg

Abstract

Data scarcity in transition metal chemistry limits the development of large-scale, general-purpose machine learning (ML) models, as tasks are problem-specific and datasets are sparse. Notable challenges include predicting chemical shifts for “exotic” nuclei such as ^{195}Pt —critical for catalysis and medicinal chemistry—and estimating activation barriers of elementary reaction steps in heterogeneous catalysis. Nanostructuring effects, such as the enhanced reactivity of edge sites¹ and low-coordinated atoms, further complicate modeling by requiring the consideration of these structural factors. Such challenges can be addressed by carefully designing model features that encode key chemical and physical properties combined with robust models such as kernel ridge regression (KRR) or gradient boosting algorithms.

In this talk, we will discuss a new ML model for ^{195}Pt NMR chemical shift prediction,² integrating Coulomb matrix elements with features like Pt atomic charge, molecular dipole moment, and integer molecular charge from fast GFN2-xTB calculations. Trained using KRR, it predicts ^{195}Pt NMR shifts in D_2O for Pt (pre)catalysts and cytotoxic Pt complexes, achieving an RMSD of 145.02 ppm (1.08% of the spectral range)—matching DFT accuracy at a fraction of the cost. Refinements that incorporate conformational, solvent, and counterion effects are underway.

For nanoparticle catalysis, we use a minimalistic descriptor framework that captures functional group reactivity and catalyst structure, combined with KRR and CatBoost, guided by newly established Brønsted-Evans-Polanyi (BEP) relationships³ tailored for catalytic networks. This enables rapid activation barrier predictions for hydrogenation, protonation, C–C bond formation, and C–O bond cleavage steps in CO_2 hydrogenation. Resulting microkinetic models link computational screening to experimental conditions, advancing predictive catalyst design.

Through data-efficient ML, we demonstrate that strategic feature engineering minimizes data requirements while preserving accuracy, enabling the prediction of molecular properties and nanoscale reactivity with practical computational tools.

Keywords: Feature engineering, machine learning, NMR chemical shifts, reaction networks, CO_2 hydrogenation

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APPLICATIONS OF SELF-ORGANIZING MAPS (SOMS) IN CHEMISTRY: FROM CLASSIFICATION TO REGRESSION

**Kanet Wongravee^{a,*}, Sureerat Makmuang^a, Nontawat Sricharoen^a,
 Thanapol Khamhla^a, and Sanong Ekgasit^a**

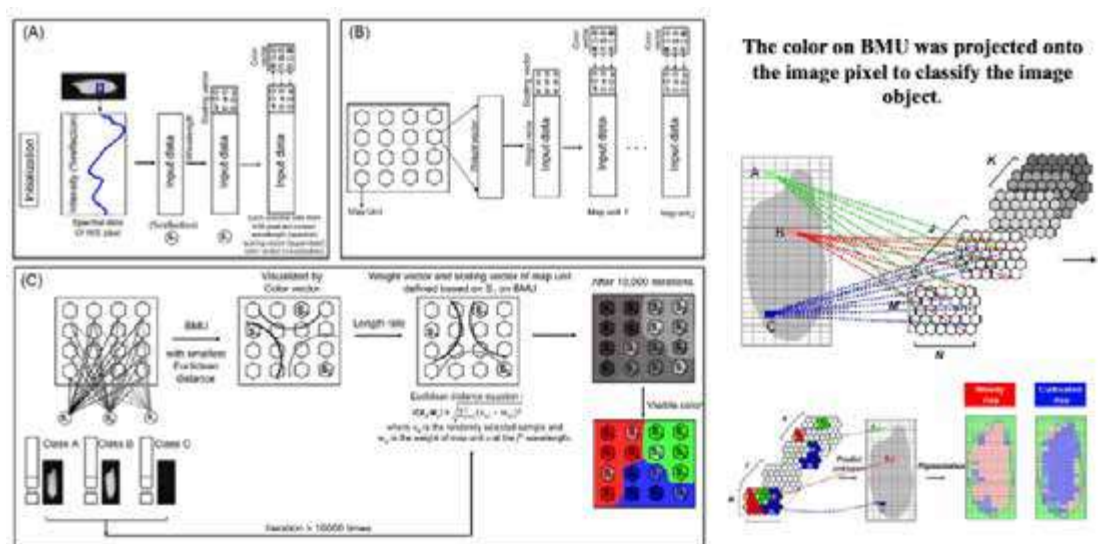
^a*Sensor Reserch Unit (SRU), Department of Chemistry, Faculty of Science,
 Chulalongkorn University, Bangkok, Thailand.*

**Corresponding author: kanet.w@chula.ac.th*

Abstract

Self-organizing maps (SOMs) have demonstrated remarkable potential in various chemometric applications, particularly in classification and predictive modeling. This work explores multiple advancements of SOMs across diverse domains, including agriculture, gemology, and material science. In agricultural applications, SOMs were optimized for classifying weedy rice from cultivated rice using near-infrared (NIR) spectroscopy, achieving high predictive accuracy (88–99%). Similarly, a modified SOM framework effectively distinguished Thai melon seed varieties, outperforming conventional discrimination models with 91.59% test accuracy. A novel approach integrating SOMs with hyperspectral imaging (HSI) further enhanced the classification of weedy rice by leveraging color indices and receiver operating characteristic (ROC) analysis, attaining accuracies of up to 98%. Beyond agriculture, SOMs were successfully applied to gemstone classification using Raman spectroscopy. A one-class SOM model, coupled with Monte Carlo permutation testing, was developed to provide robust and reliable gemstone identification, ensuring high classification confidence even for unknown samples. Expanding SOMs beyond classification, this study introduces SOM-MLP, an extension combining SOM with multilayer perceptron (MLP) for regression tasks. Applied to gold nanoparticle characterization, SOM-MLP effectively classified nanoparticle shapes and predicted surface plasmon resonance (SPR) properties, achieving mean absolute percentage errors (MAPE) of 3.82–6.72%. The framework can be further adapted to incorporate alternative regression algorithms for enhanced predictive capabilities. These advancements underscore the versatility of SOMs in chemistry, offering robust solutions for classification, pattern recognition, and predictive modeling in complex chemical datasets.

Keywords: Self Organizing Maps, Chemometrics, Hyperspectral Imaging, Near-Infrared Spectroscopy, Raman Spectroscopy



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MACHINE LEARNING FOR PROTEIN IDENTIFICATION AND BIOMARKER DISCOVERY IN MASS SPECTROMETRY-BASED PROTEOMICS

Mark V. Ivanov^{a*}, Mikhail V. Gorshkov^a

^a*V. L. Talrose Institute for Energy Problems of Chemical Physics, N. N. Semenov Federal Research Center of Chemical Physics, Russian Academy of Sciences, 119334 Moscow, Russia*

**Corresponding author: markmpt@gmail.com*

Abstract

Identification and quantification of proteins in complex samples is based on liquid chromatography (LC) and tandem mass spectrometry (MS/MS). Previously, we developed a novel method for rapid proteome analysis called DirectMS1¹. It is based on protein identification without peptide fragmentation, which distinguishes it from other traditional MS/MS-based methods and allows reducing analysis time by an order of magnitude. In the core of DirectMS1 are multiple AI-based algorithms. Specifically, gradient boosting LightGBM implemented in the method's data processing is a key for achieving its high efficiency and challenging the complexity of the problem associated with the presence of very high noise content, the need for on-the-fly learning, and the lack of reliable training samples. This algorithm is used to separate the identified peptides into groups based on their multiple measured physico-chemical properties. One of the interesting applications to be reported is finding the biological insights behind the phenomenon of Asymptomatic Alzheimer disease. We applied DirectMS1's protein search engine to a largest collection of proteomic data on post mortem human brain samples available to date. To reveal the key proteins behind the mechanism of Asymptomatic Alzheimer we also proposed and developed a ML-based workflow, aiming at improving generalizability across multiple data sets². In particular, we customized the decision tree model by introducing a new parameter, `min_groups_leaf`, which regulates the presence of the samples from each data set inside the model's leafs. Further, we analyzed a trend for feature importance's curve as a function of the novel parameter for feature selection to a list of proteins with significantly improved generalization. Our analysis resulted in the identification of two proteins that point to the ferroptosis as a key mechanism responsible for developing Alzheimer disease.

This work was performed with financial support from the Russian Science Foundation, grant no. 23-45-00012.

Keywords: mass spectrometry, proteomics, alzheimer, machine learning

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MACHINE LEARNING AIDED CHARGE TRANSPORT DYNAMICS

Chao-Ping Hsu^{a*}

^a*Institute of Chemistry, Academia Sinica, Taipei, Taiwan 11529*

^{*}*Corresponding author: cherri@sinica.edu.tw*

Abstract

Charge transport in semiconducting organic molecular solids presents unique challenges that conventional theories struggle to fully describe. Our research focuses on characterizing electron transfer coupling - specifically, the off-diagonal Hamiltonian element in diabatic state representations commonly used in polaron models. We found that this coupling exhibits high sensitivity to molecular geometries, particularly intermolecular configurations. While the nuclear dependency of this coupling plays a crucial role in charge-transport dynamics, its effects have remained largely unexplored, primarily due to computational constraints. To overcome these limitations, we developed novel machine learning (ML) approaches for evaluating electronic coupling.^[1,2,3] These ML models enabled us to investigate the spectral density function of the off-diagonal term, revealing both sub-Ohmic behavior and temperature dependence.^[4] Additionally, we examined the outer-sphere reorganization energies in nonpolar systems, which significantly influence charge transfer activation energies. Although traditional dielectric polarization theories predicted negligible outer-sphere reorganization energy, our findings demonstrate substantial contributions to this parameter.^[5] This discovery suggests that charge-transfer processes in typical nonpolar or weakly polar materials experience greater fluctuations than previously theorized models indicated. Our findings advance the fundamental understanding of charge transfer dynamics and challenge existing models in the field.

Keywords: Charge transfer, electronic coupling, machine learning, reorganization energy

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MODELING ASYMMETRIC CATALYSIS WITH MACHINE LEARNING AND STRUCTURAL FEATURES

Pavel Sidorov^{a*}, Nobuya Tsuji^a, Yuuya Nagata^a, Alexandre Varnek^{a,b}, Benjamin List^{a,c}

^a Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University.

^b Laboratory of Chemoinformatics, University of Strasbourg.

^c Max-Planck-Institut für Kohlenforschung.

*Corresponding author: pavel.sidorov@icredd.hokudai.ac.jp

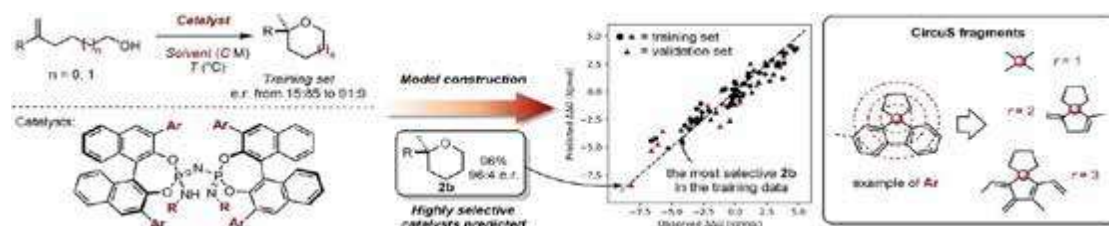
Abstract

Asymmetric catalysis is one of the most important techniques in the modern organic synthesis, allowing to guide the chemical reaction to a desired product with high efficiency. However, catalyst optimization processes typically rely on inductive and qualitative assumption of chemists based on screening data. In this work, we design new selective imidodiphosphorimidate (IDPI) catalysts¹ for hydroalkoxylation reactions² leading to the formation of tetrahydrofuran (THF) and tetrahydropyran (THP) rings with asymmetric substituents. We employ a machine learning model based on molecular fragments, which are fine-tuned for asymmetric catalysis and represent cyclic or polyaromatic hydrocarbons, enabling robust and efficient virtual screening.

To account for the complexity of the catalysts structure, which contain multiple condensed aromatic rings, as well as polycyclic substituents, we developed augmented substructure type descriptors called CircuS (**Circular Substructures**). They explicitly consider encountered full substructures with closed rings, representing complex structural motifs more specifically. The CircuS outperformed other descriptors; the fully optimized SVM regression model built on CircuS fragments of catalyst substituents demonstrated $R^2=0.905$, mean absolute error MAE=0.741 kJ mol⁻¹ in leave-one-out cross-validation in preliminary benchmark.

The final SVM regression model was built using data available for two substrates, resulting in 70 data points in total. While the model was trained using data with only moderate selectivities, we have successfully performed the virtual screening of previously experimentally untested catalysts and selected and validated experimentally new hits showing higher selectivities in a previously unaddressed transformation. The approach was also tested on literature data and has shown performance on par with state-of-the-art 3D methods³.

Keywords: asymmetric catalysis, machine learning, descriptors, molecular fragments



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RATIONAL DESIGN OF CATALYSTS ACCELERATED BY AI ASSISTED COMPUTATIONAL CHEMISTRY

Zhi-Jian Zhao^a

^aSchool of Chemical Engineering and Technology, Tianjin University, Tianjin 300350, China

^aCorresponding author: zjzhao@tju.edu.cn

Abstract

With continuous advancements in computer hardware and breakthroughs in interdisciplinary fields such as quantum mechanics, fluid dynamics, and artificial intelligence (AI), computational simulation methods have garnered significant attention for accelerating the development of industrial catalysts. Mature multi-scale computational methodologies ranging from density functional theory to continuum models have been progressively established. By employing AI-accelerated computational approaches, it becomes possible to overcome the limitations of traditional model-based catalytic systems. This enables the construction of realistic models for complex industrial catalysts under diverse reaction conditions, achieving large-scale and long-term “operational condition” simulations for industrial catalytic systems. Furthermore, by establishing structure-activity relationships of dynamic catalyst surfaces and developing reaction descriptors for rapid prediction of catalytic performance, high-throughput screening of novel catalytic materials can be realized. Intelligentized high-throughput laboratories, integrating automated experimental platforms with data-driven optimization algorithms, further accelerate the design, validation, and process development of new catalysts, significantly shortening R&D cycles and enhancing experimental efficiency.

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PREDICTING CO ADSORPTION ON MULTI-ELEMENTAL ALLOY NANOPARTICLE USING MACHINE LEARNING

Susan Meñez Aspera^{a,*}, Gerardo Valadez Huerta^a, Yusuke Nanba^a, Kaoru Hisama^a,
 Michihisa Koyama^{a,*},

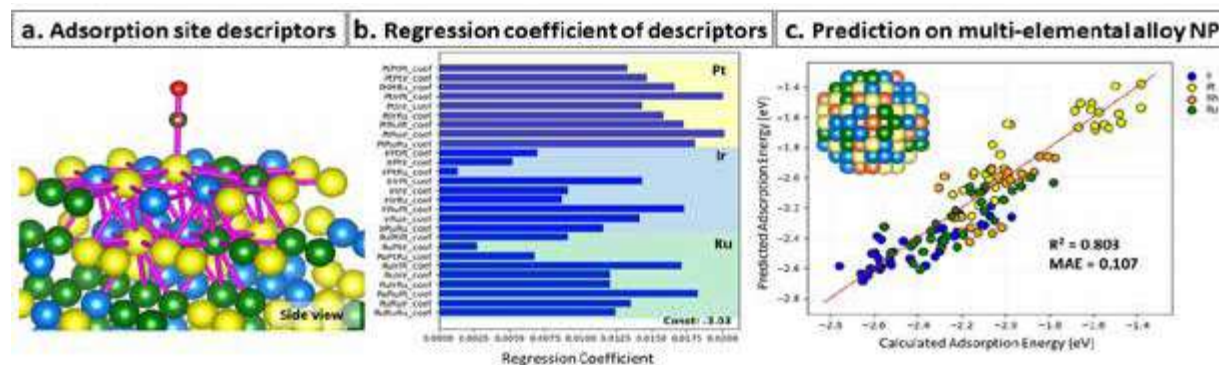
^aShinshu University

*Corresponding author: aspera_susan@shinshu-u.ac.jp, koyama_michihisa@shinshu-u.ac.jp

Abstract

Molecule adsorption on catalysts' surface is one of the foregrounds in the analysis of catalytic reactions. However, determining viable molecular adsorption sites on a multi-elemental alloy nanoparticle (NP) introduces complexity due to its multi-faceted structure and several possible elemental configurations. In this study, we applied machine learning (ML) to predict CO adsorption on platinum group metal ternary alloy NP (RuRhPt, RhIrPt, RuIrPt and RuRhIr) using our generated dataset of adsorption energies on NP alloys with varying atomic concentrations and configurations, and whose adsorption sites are described by a network of element-based neighbors inspired by the generalized coordination number^{1,2}. For fast calculation, the adsorption energies were calculated using a universal neural network potential called Pre-Ferred Potential³. Least absolute shrinkage and selection operator regression was used as a ML model to predict adsorption energies where it could allow us to determine atomic combinations in the network of elements coordinating the adsorption site that contributes to the strength of CO adsorption. The predicted and calculated values of adsorption energies were compared and evaluated using coefficient of determination (R^2) and mean absolute error (MAE). For adsorption on top sites, R^2 varies from 0.705-0.854 and MAE varies from 0.0811 eV – 0.1060 eV. Since the description of the adsorption site is a network that spans only through the neighboring atoms of the neighbor of the adsorption site, we used the information of the regression coefficients from different ternary alloy combinations to predict CO adsorption on a multi-elemental alloy NP (RuRhIrPt)⁴. This method could accelerate adsorption screening on multi-elemental alloy NP and aid in the analysis of reactions.

Keywords: Multi-elemental alloy nanoparticle, Machine learning, Generalized coordination number, Adsorption prediction, Platinum group metals



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Acknowledgement

This work was supported in part by the Ministry of the Environment, Japan "Demonstration Project of Innovative Catalyst Technology for Decarbonization through Regional Resource Recycling".

CONSTRUCTING A TEMPERATURE TRANSFERABLE COARSE-GRAINED MODEL OF CIS-1,4-POLYISOPRENE WITH PRESERVED STATIC, DYNAMIC, AND MECHANICAL PROPERTIES AIDED BY MACHINE LEARNING

Hongxia Guo ^{a,b,*}

^a *Institute of Chemistry Chinese Academy of Sciences, Beijing 100190, China.*

^b *University of Chinese Academy of Sciences, Beijing 100049, China.*

**Corresponding author: hxguo@iccas.ac.cn*

Abstract

Recently, the systematic coarse-grained (CG) model, which is a reduced but realistic representation of the chemically specific systems and allows for computationally efficiently exploring the real polymers over extended length and time scales, provides new opportunities for a full understanding of the relation between polymers' structural characteristics and material properties. However, the successful application of CG models critically relies on the development of the accurate, reliable, and computationally efficient CG force field (FF). Besides, with the rapid development of artificial intelligence, machine learning (ML) techniques have started to emerge as a promising and helpful tool in optimization of the CG FF parameters. Hence constructing a CG model to capture the static, dynamic, and mechanical properties as well as their temperature dependence of the underlying atomistic system with the aid of ML becomes a current research focus in the polymer modelling. Polyisoprene (PI) is a widely used polymer and systematic coarse-grained (CG) modelling facilitates the efficient exploration of its properties across broad length and time scales. Our research focuses on developing a systematic CG model for polyisoprene with preserved static, dynamic, and mechanical properties aided by machine learning. we present a novel approach for determining the optimal CGPI non-bonded potential parameters by coupling a Particle Swarm Optimization algorithm as the calibrator with machine learning-based models trained using molecular dynamics data. The resulting CG model is further augmented with temperature and dissipative factors through a multistate parameterization approach and friction-corrected thermostat. This enhancement ensures the model's temperature transferability of structure, thermodynamics, dynamics, and mechanics in a wide temperature of 150K~750K. The successful melding of machine learning with systematic CG molecular dynamics simulations presents a promising avenue for addressing specific polymer science problems, potentially leading to more efficient and cost-effective material design and development processes.

Keywords: machine learning, coarse-grained model, force field, molecular dynamics simulation, Particle Swarm Optimization algorithm

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MACHINE LEARNING MODELS FOR ANTIBODY-ANTIGEN BINDING AFFINITY PREDICTION: A FEATURE ENGINEERING APPROACH

Ruzanna Yahya^a, Vannajan Sanghiran Lee^{a*}, Sharifuddin Md Zin^a, Tang Wai Kit^a

^a*Department of Chemistry, Centre of Excellence in Quantum Information Science and Technology (UMQIST),
Universiti Malaya, Kuala Lumpur, 50603, Malaysia*

**Corresponding author: vannajan@um.edu.my*

Abstract

Accurate prediction of antibody-antigen binding affinity is essential for immunological research, drug development, and vaccine design. The complexity of these interactions, involving a range of molecular features, presents considerable challenges. Machine learning (ML) models offer a promising approach but require well-engineered features that capture the key molecular interactions. This study aims to create a machine learning framework based on feature engineering to predict antibody-antigen binding affinity. By combining structural, physicochemical, and sequence-based features, the goal is to enhance both prediction accuracy and model interpretability. A comprehensive set of features from antibody-antigen complexes, including sequence-based information, structural characteristics, and physicochemical properties were compiled. Machine learning algorithms like Random Forests (RF) and XGBoost were employed to classify binding and non-binding residues based on these features. To mitigate class imbalance, the Synthetic Minority Over-sampling Technique (SMOTE) was applied. Hyperparameter optimization was carried out using Bayesian Optimization to fine-tune model performance. The models achieved robust predictive performance, with XGBoost yielding the highest accuracy in predicting binding residues. The inclusion of sequence-based and structural features substantially improved prediction accuracy compared to using sequence alone. SMOTE addressed class imbalance and reduced overfitting, while hyperparameter tuning further enhanced the model's generalizability. This study demonstrates the critical role of feature engineering in antibody-antigen binding affinity prediction. By integrating sequence, structural, and physicochemical features into machine learning models, we developed a more accurate and interpretable prediction framework. Our approach is applicable to therapeutic antibody design, precision medicine, and vaccine development, offering a reliable tool for real-world applications.

Keywords: antibody-antigen, machine learning, feature engineering, binding affinity prediction,

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CHEMISTRY STUDENTS' AWARENESS OF ARTIFICIAL INTELLIGENCE (AI)- ENHANCED LEARNING

Habiddin Habiddin^{a,b,*}, Yahmin Yahmin^a

^a*Department of Chemistry, Universitas Negeri Malang, East Java, Indonesia.*

^b*Department of Science Education, Universitas Negeri Malang, East Java, Indonesia.*

**Corresponding author: habiddin_wuni@um.ac.id*

Abstract

Surveys have indicated that Indonesian students still require proper guidance to utilise artificial intelligence.^{1,2} Meanwhile, most Indonesian chemistry students struggle to extract information represented in visual phenomena, particularly when transforming visual representations into chemical behaviour.^{3,4} The emergence of Artificial Intelligence (AI) tools offers the potential to reform the chemistry education system. This paper outlines the initial efforts to gain insight into students' awareness of AI tools, including the types of AI platforms they used, their purposes, the kinds of AI that help them grasp chemistry concepts, and their familiarity with AI image explainers. Five chemistry students (fifth year) participated in the research. Data was collected using a semi-structured interview. This study revealed that all five students were familiar with various AI tools, including ChatGPT, DeepSeek AI, and Consensus AI. They primarily utilised these tools to gather necessary information for their academic assignments. Specifically, they used Consensus AI to find suitable articles for writing their theses. They agree that other sources should verify information from AI. However, the students still do not use AI to interpret visual representations in chemistry, such as graphs, diagrams, and particulate or sub-microscopic representations, like the role of catalysts in Figure 1. This research indicates that chemistry students are still not using AI tools optimally, particularly the Image explainer, which is highly advantageous for comprehending chemistry's visual and submicroscopic aspects. Due to the limited number of respondents, the results of this study cannot yet be considered representative of all Indonesian chemistry students. However, these preliminary findings highlight the need to evaluate the AI literacy of Indonesian students to help them utilise AI for academic purposes. There is an urgent need to develop AI-assisted chemistry instruction.

Keywords: AI for chemistry teaching, visual representation in chemistry, AI literacy

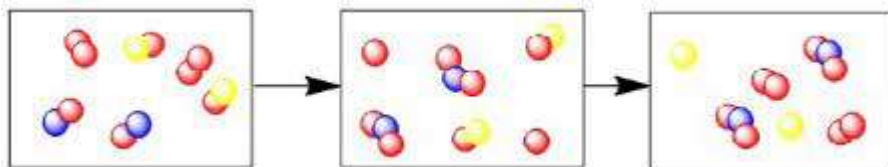


Figure 1. Catalysts role.

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MULTI-MODAL ARTIFICIAL INTELLIGENCE FOR MOLECULAR-LEVEL MAPPING OF ORGANIC - MINERAL INTERFACES IN SHALE

Xiangye Kong^{a,*}

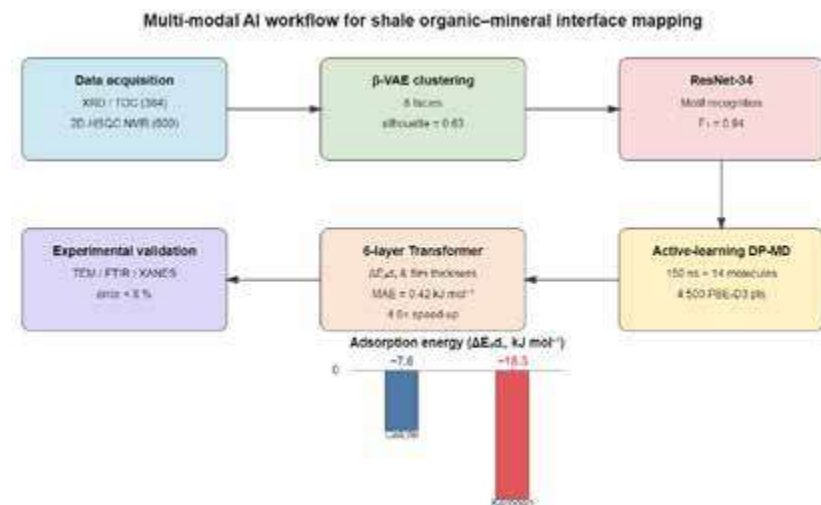
^aChengdu University of Technology, Chengdu 610059, China

*Corresponding author: kongxiangyecup@163.com

Abstract

Organic–mineral interfaces dictate hydrocarbon storage and flow in shale, yet their nanometre-scale heterogeneity hinders systematic, high-throughput characterisation. We present a reproducible, transferable workflow that couples experiments, molecular simulation and multi-modal artificial intelligence to quantify interfacial chemistry, adsorption energetics and film architecture in real shale systems. β -Variational auto-encoder clustering compresses 384 powder-XRD/TOC profiles from four Chinese basins into eight mineral–kerogen facies (silhouette = 0.63); a ResNet-34 classifies 600 high-field 2D-HSQC NMR spectra ($F1 = 0.94$) to identify molecular motifs; active-learning Deep-Potential models trained on 4500 PBE-D3 reference structures drive 150 ns NVT molecular dynamics for 14 C6–C30 organics on calcite, illite and type-II kerogen; and a six-layer Transformer regressor predicts adsorption energies (ΔE_{ads}) and multilayer thicknesses from 12000 interfacial configurations, delivering a mean absolute error of 0.42 kJ mol⁻¹ and a 4.6-fold speed-up over PBE-D3 while retaining 93.8 % accuracy. Predicted ΔE_{ads} span weak physisorption on calcite (-7.6 ± 1.2 kJ mol⁻¹) to strong π – π stacking on kerogen (-18.3 ± 1.5 kJ mol⁻¹), with adsorption layers 1.90–2.89 nm thick; attribution analysis shows aromatic-N and organosulfur groups dominate clay binding, whereas branched aliphatics preferentially populate kerogen nanopores. High-resolution TEM, in-situ FTIR and C-K-edge XANES measurements validate the AI predictions within 8 % across 298–373 K and 0.1–1.3 M salinity. The resulting framework enables rapid, quantitative mapping of organic–mineral interfaces in shale and is readily extensible to catalytic oxides, geothermal brines and CO₂ storage horizons.

Keywords: multi-modal artificial intelligence, shale, adsorption energy, molecular dynamics, graph neural network



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ARTIFICIAL INTELLIGENCE IN AGRICULTURAL CHEMISTRY AND AGRICULTURE

Bipul Behari Saha

Shree Chaitanya Education Society

**Corresponding author: drbsaha@rediffmail.com*

Abstract

Artificial Intelligence is finding extensive application in Agricultural Chemistry and Agriculture. This includes cost effective discovery of new crop protection chemicals like fungicides and herbicides and fast development of synthetic route of agrochemicals. A.I. is also used in formulation development of crop protection chemicals to forecast emulsion stability, dispersion rate and other physical properties. Another very important application of A.I. is prediction of toxicity of new molecules which are in R&D stage. If it is predicted that new molecule will have high toxicity, then there is no need to waste time for developing such molecules. Artificial Intelligence is also helping farmers in India in multiple ways such as prediction of right time to sow seed, early diagnosis of plant diseases, selective removal of weeds by intelligent spraying, monitoring of soil quality and crop health etc. Details will be discussed.

Keywords: A.I., Agricultural Chemistry, Agriculture, Plant disease diagnosis, Discovery research

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MACHINE LEARNING ASSISTED IN UNCOVERING MOLECULAR DESIGN PRINCIPLES FOR THE DEVELOPMENT OF MULTIPLE-RESONANCE TADF EMITTERS

W. K. Tang*, C. H. Ng, M. Ng, Y. Wang, S. N. Saw, S. S. Chen, M.-C. Tang

Department of Chemistry, Universiti Malaya

**Corresponding author: wktang@um.edu.my*

Abstract

Third-generation organic light-emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) offer enhanced efficiency by converting non-emissive triplet excitons to emissive singlet excitons via reverse intersystem crossing (RISC). Minimizing the singlet-triplet energy gaps (ΔE_{ST}) while maintaining desirable emission energy is critical for advancing OLED opto-electronic applications. Among TADF emitters, multiple-resonance TADF (MR-TADF) compounds have gained significant attention due to their narrow emission bandwidths and high color purity, making them ideal candidates for next-generation OLEDs. Traditionally, the development of efficient RISC in stable MR-TADF emitters relies heavily on experimental synthesis, which is both time-consuming and resource-intensive. Machine learning provides a cost-effective alternative to uncover structure-property relationship and guide the design of novel MR-TADF materials prior to synthesis. Here, we present a machine learning (ML)-guided strategy to decode molecular design principles and accelerate the discovery of efficient double-boron MR-TADF materials. A database of over 327 MR-TADF molecules with corresponding ΔE_{ST} was constructed and transformed into numerical features via feature engineering method. Various ML algorithms were trained to predict the ΔE_{ST} with the XGBoost model exhibiting the best performance, achieving an R^2 value of 0.71 and the highest accuracy. Our ML model reveals that the ΔE_{ST} is influenced by factors such as extended π -conjugation, the presence of three-single-bonded boron and nitrogen atoms which facilitate charge transfer (CT) properties. Utilizing these insights, we performed large-scale predictions based on a BN-core scaffold to refine the molecular design strategies on the scaffold and identified a promising double-boron, DPAC-DB. Experimental validation of DPAC-DB confirmed the effectiveness of our ML-guided design strategy: the emitter exhibited a significantly reduced the ΔE_{ST} of 0.14 eV and an enhanced the rate of RISC of $1.12 \times 10^5 \text{ s}^{-1}$. As a blue-emitting material, DPAC-DB also demonstrated excellent device performance, achieving a maximum external quantum efficiency (EQE) of 35.6% with a reduced efficiency roll-off of 24% at 1000 cd m^{-2} . Our works successfully developed a robust ML-assisted paradigm for rational design of double-boron MR-TADF materials to advance stable and high-efficiency OLEDs.

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EMPOWERING CHEMISTRY EDUCATION: GREEN CHEMISTRY AND SUSTAINABLE DEVELOPMENT IN SOUTH AND SOUTHEAST ASIA

Supawan Tantayanon^{a,*}

^a*Department of Chemistry, Faculty of Science, Chulalongkorn University.*

^{*}*Corresponding author: supawan.t@chula.ac.th*

Abstract

The integration of green chemistry principles into education plays a crucial role in advancing Sustainable Development. This keynote presentation will highlight innovative approaches to chemistry education in South and Southeast Asia, with a focus on small-scale chemistry experiments that promote sustainability, safety, and cost-efficiency. It will explore the transformative “Dow Chemistry Classroom” initiative, launched in Thailand in 2014, which introduced a groundbreaking model of teaching science by conducting hands-on laboratory experiments directly within high school classrooms.

The session will discuss how these educational innovations align with the broader goal of enhancing scientific and technological understanding for sustainable development and fostering scientific literacy among students. Through workshops and training programs, educators are empowered to design and implement experiments that minimize waste, promote safety, and adhere to the 12 principles of green chemistry. This hands-on approach not only improves the learning experience but also equips high school teachers to become catalysts for change, creating networks of trained educators who share knowledge and resources across the region.¹

The presentation will reflect on the successes, challenges, and key lessons learned from these educational initiatives, illustrating how green chemistry-based methods contribute to sustainable development.² It will also highlight IUPAC’s commitment to addressing global challenges, especially in advancing SDG 4 (inclusive and equitable quality education) through multidisciplinary educational projects. By empowering educators and fostering cross-border collaboration, these efforts contribute to building a more sustainable, scientifically literate future for South and Southeast Asia, aligning with IUPAC’s mission to provide expertise that addresses critical world needs.

Keywords: green chemistry, sustainable development, small scale chemistry

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GREEN CHEMISTRY IN EDUCATION: A MODEL FOR SUSTAINABLE CHEMISTRY TEACHER TRAINING AND CURRICULUM INNOVATION

Mageswary Karpudewan

School of Educational Studies, Universiti Sains Malaysia

Corresponding author: kmageswary@usm.my

Abstract

Chemistry is often regarded as the “mother of all sciences” because it forms the foundation for various industrial and manufacturing sectors. Advancements in chemistry have significantly contributed to medical breakthroughs, extending human longevity, and have played a crucial role in engineering innovations that enhance the quality of life. However, traditional chemistry relies heavily on hazardous and harmful substances, leading to adverse consequences for human health and the environment. If these challenges are not addressed at an early stage, they can result in long-term social and economic problems.

Green Chemistry, which emerged in the 1990s as a sustainable alternative to conventional chemistry, has been increasingly adopted by industries to minimize environmental impact. While the widespread application of Green Chemistry principles in industries is commendable, integrating Green Chemistry into the education system—starting from high school—can create a strong foundation for students to understand chemistry in relation to environmental, economic, and societal sustainability.

In this context, teacher education and training play a vital role in fostering sustainable chemistry education. Introducing pre-service and in-service chemistry teachers to Green Chemistry and equipping them with pedagogical strategies to teach chemistry through a sustainability lens can facilitate the transition from conventional to sustainable chemistry at the school level. This presentation highlights various initiatives undertaken at the School of Educational Studies, Universiti Sains Malaysia, to educate and train chemistry student teachers in Green Chemistry. These efforts are expected to provide a model for others to adopt and implement similar approaches within their own educational contexts.

Keywords: Green Chemistry in Education; Model; Pedagogy; Teacher Training

BEYOND THE 12 PRINCIPLES: ASKING INSTRUCTORS TO MODERNIZE THEIR CURRICULA

David A. Laviska*

American Chemical Society Green Chemistry Institute

**Corresponding author: d_laviska@acs.org*

Abstract

In 2023, the American Chemical Society formalized guidance for chemistry degree programs that features well-defined requirements for the inclusion of green chemistry, systems thinking, and case studies throughout the chemistry curriculum. While this update to ACS guidelines underlines the urgent need to modernize our curricula, it is important to acknowledge that curricular change is fraught with challenges and tends to happen slowly, if at all. Most of the effort and time required to update and/or change curricular components falls on instructors who may themselves need to expand their thinking and/or learn new concepts and skills before taking on the responsibility for training students. At the ACS Green Chemistry Institute, we have been working for several years on developing free, open-access teaching modules that incorporate green and sustainable chemistry across standard undergraduate curricular topic areas. More recently, we have launched multiple faculty mentoring networks (FMNs) to support instructor collaboration and training at all levels of teaching/learning. We have also developed a self-guided “case study template” that will enable instructors to creatively take examples of “real-world chemistry” into their classes. In this talk, I will discuss our efforts to support instructors and invite attendees to collaborate with us as we work together toward curricular change.

Keywords: Green Chemistry, Curricular change, Faculty support, Professional development, Case studies

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PROMOTING A SYSTEMIC CHANGE IN CHEMISTRY EDUCATION: BEYOND BENIGN AND THE GREEN CHEMISTRY COMMITMENT

Juliana Vidal^a, Natalie O'Neil^a, Omar Villanueva^a, Amy Cannon^{a,*}

^a*Beyond Benign, 18 Church Street, 1016, Wilmington, MA, USA*

^{*}*Corresponding author: amy_cannon@beyondbenign.org*

Abstract

Green chemistry education is a fundamental approach to achieving a sustainable future and creating long-lasting and impactful change in our society. Integrating green chemistry into the curricula promotes the development of scientists with the required skills to assess and design safer and benign processes and products for human health and the environment. To catalyze and support this inclusion, Dr. Amy Cannon and Dr. John Warner co-founded Beyond Benign in 2007. Beyond Benign is a non-profit organization that works across the education continuum to empower the chemistry community to practice sustainability at the molecular level through green chemistry. One of its initiatives at the higher education level is the Green Chemistry Commitment (GCC), a collective voice of institutions, universities, and colleges worldwide committed to integrating green chemistry into their educational systems. Over 220 higher education institutions from over 25 countries are a part of the GCC program, and their work is based on unique campus environments, strengths, cultures, and resources. In this presentation, the impact of the GCC program and the approaches taken by the participating institutions will be highlighted, as well as the systemic benefits of integrating green chemistry principles and practices in education toward a sustainable, safer, and greener future for our society and beyond.

Keywords: Green chemistry, education, sustainability.

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NOVEL ENVIRONMENTALLY FRIENDLY HYDRO-INDUCED FADING DYES IN WRITING AND PAINTING APPLICATIONS

Jiayang Feng^a, Dan Chang^a, Chuan Dong^a, Shaomin Shuang^{a*}

^aShanxi University, PR China

*Corresponding author: smshuang@sxu.edu.cn

Abstract

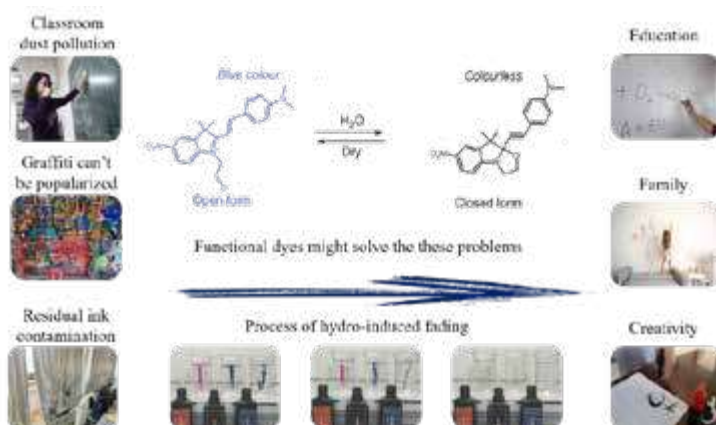
Dyes are the coloring agents of human civilization, yet the quest for color has always come with a hidden cost to the environment¹. Our team developed hydro-induced fading dyes to create sustainable writing and painting solutions, addressing pressing environmental and health concerns in traditional pen products. The dyes, when exposed to water, fade rapidly into colorless and leaves no trace. Unlike conventional inks, which often contain toxic solvents like benzene and alcohol², our dyes are non-toxic, odorless, and SGS-certified, complying with ASTM F963-11 and EN71-3 safety standards.

The key applications include:

1. Education: Dust-free teaching pens that promote healthier classroom environments by eliminating dust-related health risks.
2. Family: Safe graffiti pens that inspire children to unleash creativity on any surface, such as walls or tables, without harmful residue or cleanup concerns.
3. Creativity: Eco-friendly art dyes that address the challenges of cleaning and environmental pollution in traditional painting practices.

This revolutionary technology has been successfully implemented in schools across China, earning widespread approval from educators and students alike. We will further explore the application of the dyes in temporary stamps, nail art, coloured bubbles, anti-counterfeiting printing, temporary hair dyes and more.

Keywords: hydro-induced fading dyes, sustainable teaching tools, eco-friendly ink, safe graffiti pen



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INNOVATION IN SUSTAINABLE DEPOLYMERISATION: AN UNDERGRADUATE LAB'S APPROACH TO GREEN CHEMICAL POLYMER RECYCLING

Rebecca L. Jones^{a,*}, Benji Fenech-Salerno^a and Laura Patel^a.

^aDepartment of Chemistry, Imperial College London, South Kensington, SW7 2AZ.

*Corresponding author: rebecca.jones@imperial.ac.uk

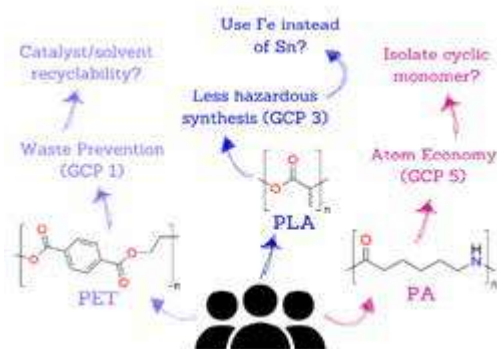
Abstract

Single-use polymers have become ubiquitous to the modern-day lifestyle. Their omnipresent nature, coupled with poor after-use disposal mechanisms, has led to a distressing accumulation of these materials in landfill sites and as pollutants in the environment. This release of harmful chemicals poses significant ecological and health risks. A report by Gayer emphasises the urgent need for sustainable polymer waste management solutions as it estimates that of the 8300 million metric tonnes of plastic produced between 1950–2015, 79% was disposed of in landfills, 12% was incinerated and only 9% was completely, and cleanly, recycled.¹

To raise awareness of this critical real-world issue, and to increase the integration of sustainability concepts into the undergraduate curriculum, an interdisciplinary experiment was recently developed. Throughout this two-week undergraduate practical, students leveraged generative AI to design sustainable depolymerisation pathways for an assigned common polymer. They were tasked with ensuring that their approaches aligned with the 12 Green Chemistry Principles (GCPs) and the UN Sustainable Development Goals. To obtain a post-consumer sample for testing, the students first had to identify their designated material from a selection of unknowns using a near-infrared identification tool. They then experimentally tested their devised depolymerisation pathways; these often incorporated low temperatures, catalysts, and/or ionic liquids. An extension of the lab allowed students to explore aspects of interest to them; common investigations included optimising reaction conditions, monomer functionalisation, and testing repolymerisation strategies.

This talk will discuss the design of this inquiry-based laboratory framework, with a primary emphasis on the synthetic component. It will highlight the integration of pedagogical approaches such as authentic assessment, (social) constructivism, and Bloom's taxonomy. Additionally, it will explore how the project fosters the development of essential circular economy practices in future STEM graduates, alongside insights into the students' experimental outcomes and their evaluation of the interdisciplinary research experience.

Keywords: inquiry-based undergraduate experiment, chemical polymer recycling, sustainability, generative AI, pedagogy.



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INTEGRATING GREEN CHEMISTRY AND MICROSCALE PRACTICES IN SCHOOLS: EXPLORING NATURAL ACID-BASE INDICATORS

Nisha Pandey^a, Shreesha Bhat^a, Ashutosh Bhakuni^a, Amarjeet Bhardwaj^a, Manish Jain^a

^aCenter For Creative Learning (CCL), Indian Institute of Technology Gandhinagar (IITGN), India;

*Corresponding author: ccl@iitgn.ac.in

Abstract

Green chemistry aims to reduce harmful chemicals and protect the environment,¹ while microscale chemistry provides opportunities to conduct experiments in a safer, cost-effective and eco-friendly manner ² as well as help achieve the UN's Sustainable Development Goals. ³ However, in the Indian context, there are few published efforts and resources on green and microscale chemistry for schools, and adequate in- service teacher training in this area through hands-on activities remains poorly addressed.⁴ Even the National Curriculum Framework for School Education based on the National Education Policy 2020 emphasises responsibility and sustainability in environment education, but misses out on the opportunity to make green chemistry an important pillar of chemistry education.⁵ At CCL we have developed several microscale chemistry education modules. This work presents an acid-base module using natural indicators like periwinkle flowers, purple cabbage, beetroot and turmeric in an effort to incorporate local resources in green chemistry education. pH profiles of natural extracts were developed and activities using these natural indicators such as indicator droplet art, neutralisation reactions, and rainbow fizz were optimised. We have tested these activities with government school students and teachers in India through various modes of delivery over a period of one year. The online sessions reached approximately 85,000 girls students from 932 schools in two states who belong to extremely disadvantaged communities.⁶ These sessions incorporated hands-on activities, polls to assess engagement and assignments with observation sheets. The enthusiasm was visible in the responses received, including homework submissions, challenge questions, and participation in science exhibitions. Teacher training workshops were conducted in-person for approximately 600 teachers from six states, and incorporated experiment kits, quizzes, observation sheets, and discussions. During workshops, teachers exhibited high engagement, finer observations, and the motivation to implement the activities in classrooms due to their safety, ease and accessibility.

Keywords: Acid Base, Green Chemistry, Hands-on Activities, Microscale Chemistry, Natural Indicators.

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THE EFFECTIVENESS OF THE ORGANIC CHEMISTRY METACOGNITIVE INSTRUCTION (OCHEM-MI) FRAMEWORK IN ENHANCING MATRICULATION STUDENTS' MECHANISTIC REASONING AND SELF-EFFICACY BELIEFS IN CHEMISTRY

Byron MC Michael Kadum

Universiti Sains Malaysia

Corresponding author: byron.kadum@student.usm.my

Abstract

Many Malaysian matriculation programme students struggle with organic chemistry concepts. Recent research underscores difficulties applying mechanistic reasoning, often relying on memorisation¹. This study advocates tailored teaching strategies to enhance comprehension. The Organic Chemistry Metacognitive Instruction (OCHEM-MI) Framework merges two metacognitive strategies—think-aloud (TA) and science writing heuristic in green and sustainable chemistry context (SWH-GSC)—to optimise learning. Integrating TA and SWH-GSC enhances organic chemistry understanding by leveraging effective metacognitive elements²: metacognition class, expert modelling, verbalisation, prompts, peer collaboration, write-to-learn, and reflection. Drawing from activity theory, conceptual understanding, metacognition theory, and self-efficacy theory, this approach aims to improve matriculation students' mechanistic reasoning (MR) and self-efficacy (SE) beliefs in chemistry. The OCHEM-MI Framework significantly enhanced students' MR. In the experimental group (EG), non-responses dropped from 80.65% to 2.42%, while causal mechanistic reasoning increased from 0.00% to 20.16%. EG students demonstrated greater accuracy in explaining reaction mechanisms, including Markovnikov's and Saytzeff's rules, electron movement, and intermediate stability. In contrast, the control group (CG) showed minimal improvement, with 64.06% still unable to provide post-test responses. The framework effectively guided students toward normative reasoning, deeper causal explanations, and mechanistic understanding, reinforcing its role in enhancing organic chemistry comprehension. Similarly, the framework significantly improved matriculation students' SE. Statistical analyses (MANCOVA and ANCOVA) revealed that EG outperformed the CG in post-test scores for SE and its constructs: SE for cognitive skills and SE for everyday applications, with small-to-medium effect sizes. Bayesian tests confirmed these findings. Qualitative analysis supported this, showing EG students showed higher confidence, adaptability, and engagement in higher-order thinking. They demonstrated innovative problem-solving, theory-practice integration, and real-life chemistry applications, prioritising sustainability. CG students relied on repetition and exhibited a surface-level understanding. Thus, the OCHEM-MI Framework is proven effective in improving matriculation students' organic chemistry MR and SE in chemistry.

Keywords: OCHEM-MI Framework, mechanistic reasoning, self-efficacy beliefs in chemistry, green & sustainable chemistry

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DEVELOPMENT OF DIY BIOPLASTIC FROM FOOD WASTE AS A SUSTAINABLE ALTERNATIVE TO SYNTHETIC POLYMERS

Nik Norhasrina binti Nik Din^{a,*}, Mageswary a/p Karpudewan^a, Nur ‘Ainiza binti Nuruddin^a

^aUniversity of Science Malaysia

*Corresponding author: hasrinanik@gmail.com

Abstract

Plastic pollution is a growing environmental concern, necessitating the development of biodegradable alternatives derived from renewable resources. This study investigates the potential of food waste such as banana peels, potato starch and orange peels as raw materials for bioplastic production. The bioplastic was synthesized by combining starch-based food waste with acetic acid (vinegar) and glycerol, followed by controlled heating and drying. The role of glycerol as a plasticizer in enhancing flexibility and mechanical properties was examined, demonstrating its ability to reduce brittleness and improve elasticity. The bioplastic samples were tested for tensile strength, flexibility and biodegradability through decomposition analysis in soil and water. Results indicate that food waste-derived bioplastics offer promising mechanical properties and faster degradation rates compared to conventional plastics, making them viable alternatives in sustainable materials research. This study highlights the significance of waste valorization in circular economy practices and encourages further exploration of bioplastics in educational and industrial applications.

Keywords: Bioplastic, food waste, glycerol, biodegradable plastic, waste valorization.

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BRIDGING STEM AND SUSTAINABILITY: THE ROLE OF GREEN CHEMISTRY IN PRIMARY EDUCATION

Sarimilla a/p Jiwathnam, Mageswary Karpudewan

^AUniversiti Sains Malaysia

Corresponding author: sarimilla.j@student.usm.my

Abstract

Integrating green chemistry principles into STEM education at the primary school level is crucial for fostering early sustainability awareness and promoting responsible scientific practices. This study examines how primary school STEM teachers incorporate green chemistry concepts into their lessons to encourage eco-conscious decision-making among young learners. By introducing non-toxic materials and waste reduction strategies, teachers can cultivate an understanding of environmental responsibility from an early age. Using a qualitative approach, data was collected through interviews and classroom observations with primary STEM teachers to examine their understanding, teaching strategies, and challenges in implementing green chemistry. The findings reveal that while teachers acknowledge the importance of sustainability in STEM education, limited resources and a lack of professional development hinder effective implementation. This study underscores the need for teacher training programs, accessible teaching materials, and curriculum support to enhance sustainability education. By embedding green chemistry into STEM teaching, students can develop a strong foundation in environmental responsibility and fostering a generation dedicated to sustainable solutions. The study highlights the need for teacher training programs, accessible teaching materials, and curriculum support to enhance sustainability education. By embedding green chemistry into STEM teaching, students can develop a strong foundation in environmental responsibility and fostering a generation committed to sustainable solutions.

Keywords: Green Chemistry, STEM Education, Primary School, Sustainability, Teacher Practices

THE EFFECTIVENESS OF GREEN SUSTAINABLE CHEMISTRY INFUSED MACHINE LEARNING ON S-TPACK, CIRCULAR ECONOMY AND SYSTEM THINKING OF IPG PRE-SERVICE TEACHERS

Deva Nanthini Sinniah

Universiti Sains Malaysia

Corresponding author: devananthinisinniah@gmail.com

Abstract

Under the Global Action Programme (GAP), the Malaysian Ministry of Education (MOE) has strengthened educators' and trainers' capacity to deliver Education for Sustainable Development (ESD). To support this initiative, Green Sustainable Chemistry (GSC) integrated with Machine Learning (ML) has been incorporated into teacher training pedagogy. GSC-ML plays a crucial role in teaching and learning acid-base chemistry, providing pre-service teachers (PSTs) with a comprehensive understanding of its function as a pedagogical tool. Through this approach, PSTs are able to acquire knowledge of S-TPACK, an expansion of the TPACK framework. TPACK introduces technology into pedagogical knowledge, but it is not adequate to ground the pedagogy in sustainability. Hence, there is a need to extend the TPACK framework by incorporating sustainability (S), forming S-TPACK, to educate PSTs on using GSC-ML as an instructional strategy. This research also evaluates PSTs' knowledge of Circular Economy (CE) and System Thinking (ST), with GSC-ML serves as a valuable pedagogical tool. The three pillars of CE—eliminate, circulate, and regenerate are essential for sustainability. By applying GSC-ML, this study aims to facilitate a shift from a linear to a circular model. Incorporating ST helps manage the complexity of scientific concepts while maintaining a holistic view of key subsystem and the intended and unintended consequences. Using a quasi-experimental design and MANOVA, this study assesses how GSC-ML enhances PSTs' application of S-TPACK and understanding of CE and ST. By fostering environmentally conscious educators, this research aims to advance sustainability-focused teaching methodologies and support Malaysia's vision for a sustainable future.

Keyword: Green Sustainable Chemistry, Machine Learning, Circular-Economy, S-TPACK, System Thinking

DEVELOPING AND VALIDATING INSTRUMENTS ON SYSTEMS THINKING AND CIRCULAR ECONOMY FOR CLIMATE CHANGE AND GREEN CHEMISTRY EDUCATION

Pavitra Krishnan^{a*}, Mageswary Karpudewan^a

^a*School of Educational Studies, Universiti Sains Malaysia*

^{*}*Corresponding author: pavitra@smskb.edu.my*

Abstract

Climate change, driven by human activities such as fossil fuel consumption, deforestation, and industrial emissions, presents significant environmental challenges. Addressing these challenges requires an education system that fosters systems thinking (ST), circular economy (CE), and green chemistry. ST helps to understand the complex interactions within the climate system; CE emphasizes waste reduction and resource efficiency; and green chemistry aims to minimize pollution and hazardous substances. Teachers, as key facilitators in education, must not only grasp these complex systems but also integrate sustainable solutions into their teaching. However, despite the growing emphasis on ST and CE in education, no specific instrument currently exists to assess teachers' knowledge in these areas. This study focuses on developing and validating questionnaires to measure teachers' systems thinking (ST) and circular economy (CE) for climate change. This exploratory mixed-method study aims to explore the subsystems of climate change and circular economy principles. Document analysis identified the subsystems as Earth's subsystems, human activities, governance, and the causes and effects of climate change, while further exploring the principles of eliminating waste and pollution, keeping products and materials in circularity, and regenerating nature. Subsequently, a 55-item questionnaire was developed for ST and a 28-item questionnaire for CE. The results of the exploratory factor analysis (EFA) revealed four distinct factors for ST and three factors for CE. A confirmatory factor analysis (CFA) was conducted to further refine and validate the questionnaires. The CFA results indicated that all four factors for ST were retained, while 30 items were removed; for CE, three factors were retained, and eight items were removed. Consequently, the final ST questionnaire comprises 25 items, whereas the CE questionnaire consists of 20 items. The findings of this study are anticipated to provide a reliable tool for assessing ST and CE within climate change and green chemistry education.

Keywords: systems thinking, circular economy, instrument development, climate change education (CCE), green chemistry education (GCE)

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IMPLEMENTATION OF A GSC-ROBOTIC APPROACH TO ENHANCE ENERGY LITERACY (EL), COMPUTATIONAL THINKING (CT) AND SUSTAINABILITY COMPETENCE (SC) OF SECONDARY SCHOOL STUDENTS

Rennukka Mathava

Universiti Sains Malaysia

Corresponding author: rennukkamahava@gmail.com

Abstract

Green and Sustainable Chemistry (GSC) emphasizes a systems-based, interdisciplinary approach to overcoming the limitations of teaching science in isolation. GSC plays a pivotal role in enhancing students' understanding of sustainable energy solutions, which can promote energy literacy (EL) by embedding sustainable practices and principles into the science curriculum. Additionally, integrating sustainable development into education can strengthen computational thinking (CT) by fostering high-impact problem-solving and decision-making skills in students. To date, the effectiveness of Education for Sustainable Development (ESD) has been assessed by evaluating students' sustainable competencies (SC). However, the relationship between GSC, EL, CT, and SC among secondary school students—both nationally and internationally—has been rarely studied. Despite its importance, GSC is not given much consideration in the IGCSE curriculum. Since implementing GSC requires interdisciplinary approaches, robotics education will be utilized as a tool to enhance EL, CT, and SC among secondary school students.

Keywords: green and sustainable chemistry, energy literacy, computational thinking, sustainable competencies, robotic education, interdisciplinary

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ASSESSING STUDENT KNOWLEDGE OF GREEN CHEMISTRY: DEVELOPMENT AND EVALUATION OF SELECTED- AND CONSTRUCTED-RESPONSE APPROACHES

Alexey Leontyev^{a,*}, Krystal Grieger^a

^a*Department of Chemistry, North Dakota State University*

^{*}*Corresponding author: Alexey.leontyev@ndsu.edu*

Abstract

Driven by the urgent need to address global environmental challenges, the integration of green chemistry into university curricula is steadily increasing. However, educators still face a critical challenge: assessing students' understanding of green chemistry principles in the absence of validated assessment tools. To address this gap, we explored two different approaches to measuring student learning—selected-response and constructed-response questions. For the selected response approach, we designed the Assessment of Student Knowledge of Green Chemistry Principles (ASK-GCP) instrument [1]. We evaluated its sensitivity and effectiveness for measuring student knowledge of green chemistry. The instrument proved to be sensitive to distinguish known groups with various levels of green chemistry knowledge and different levels of instructional exposure to green chemistry. The instrument detected gains in green chemistry knowledge in pre- and post-condition. However, one of the disadvantages of selected-response questions is their limited ability to provide insights into student misconceptions and reasoning. We utilized constructed-response case comparison prompts to address this problem and elicit their reasoning about green chemistry. We incorporated a series of two-reaction case comparison prompts within organic chemistry lectures and laboratory courses to evaluate student knowledge and application of green chemistry principles. In these prompts, two reaction alternatives were represented, and students were asked to identify which of two reactions would be the “greener” option and explain their reasoning [2]. In addition, we also investigated the functioning of a non-content-based prompt which was found to be suitable as a pre-test for students at the beginning of organic chemistry classes. All versions of case comparison prompts are instrumental in measuring students' argumentation skills. The presentation will share our findings on assessment design, outline practical steps for implementing assessments in chemistry curricula, and invite international collaborations to examine how these assessments function in diverse instructional settings worldwide.

Keywords: Green Chemistry, Assessment, Evaluation of Knowledge

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WHAT CHEMISTRY TEACHERS ARE THINKING: LEANING GREEN WHEN CONDUCTING PRACTICAL ACTIVITIES

Seamus Delaney^{a,*}, Madeleine Schultz^b

^a School of Education, Deakin University, Australia.

^b School of Life and Environmental Sciences, Deakin University, Australia.

*Corresponding author: s.delaney@deakin.edu.au

Abstract

Chemistry educators across the globe incorporate hands-on activities into their teaching for a variety of purposes. However, in many countries, there is limited information about what exactly teachers do during laboratory sessions and to what extent they incorporate green chemistry or sustainability-related activities. To address this lack of knowledge, a comprehensive international survey was recently launched¹, aimed at gathering extensive baseline data by asking high school teachers about the types and frequency of practical activities they use in their classrooms, including those related to green and sustainable chemistry (GSC). The survey was initially designed based on literature discussing teachers' objectives for practical activities^{2,3}. The core of the survey focuses on the frequency, perceived importance, and barriers to practical activities, capturing what *teachers are actually doing* in classrooms. At the end of the survey, teachers are also asked if they have a GSC-related practical activity that they would like to share with teachers globally. In this presentation, we will present a preliminary analysis of the collected results from all participating countries (as of March 2025, around 10,500 valid responses from 57 countries and in 37 languages). Regional factors, such as educational policies, curriculum priorities, and resource availability, may influence teacher adoption of GSC practical activities in schools. The potential of these findings to guide teaching practices, inform professional development programs, and foster curriculum innovation will also be evaluated and discussed. The authors have many people to thank for their ongoing involvement in this project, who have acted as country coordinators in the 57 countries (as of March 2025) where the survey has been implemented. Funding for this project was provided by the International Union of Pure and Applied Chemistry (IUPAC). The authors thank the IUPAC Committee on Chemical Education for their support.

Keywords: green and sustainable chemistry, schoolteachers, practical activities, survey

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INTEGRATING GREEN TECHNOLOGY AND CUTTING-EDGE RESEARCH INTO UNDERGRADUATE LABORATORY COURSES FOR INNOVATIVE TALENTS

Lingling Li*

Department of Chemistry, University of Science and Technology of China, 96 Jinzhai Rd, Hefei, 230026.

*Corresponding author: lill09@ustc.edu.cn

Abstract

We integrate green chemistry into laboratory courses from multiple aspects, including virtual simulation experiments (VSE), transformation of major research achievements into new teaching contents, and course-based undergraduate research experiences (CUREs). This effort aims to cultivate top-tier undergraduate talents efficiently. The following are some specific implementation strategies. (1) Friedel-Crafts acylation is one of the laboratory teaching topics widely conducted in colleges and universities today, among which acyl halides or acid anhydrides are often used as acylating agents. However, their preparation and use create significant chemical waste and pose safety issues. Herein, we introduce BHC ibuprofen process and an unprecedented green synthetic strategy using CO as a carbonyl source in our organic laboratory course^[1]. This enables students to master the atom economy in green chemistry and stay informed about current industrial green processes and important cutting-edge achievements related to textbook knowledge^[2]. (2) We transform the revolutionary breakthrough in crystallography, the crystalline sponge method, into new content for undergraduate laboratory course. Students are guided to explore low-toxicity alternative reagents for that used in the groundbreaking work of the crystalline sponge method. This integrates green chemistry with breakthrough technology in the classroom^[3, 4]. (3) In analytical chemistry laboratory, chromium is a common laboratory waste. We implement CUREs on new strategies for the green treatment of chromium-containing wastewater, which strengthens students' research practices in green chemistry. Our work won the Grand Prize in the National Chemistry Experiment Innovation and Design Competition for College Students. The findings were published in Journal of Chemical Education, and achieved top 5% of all research outputs by Altmetric. In addition, we were honored with Provincial-Level First-Class Course.

Keywords: Green Chemistry, Undergraduate Laboratory Courses, Virtual simulation experiment, Integration of Major Scientific Research Achievements, CUREs



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THE DIFFERENTIATED INSTRUCTION- GREEN CHEMISTRY APPROACH: AN ALTERNATIVE APPROACH REFLECTING ON INCLUSIVITY FOR INTERNATIONAL GENERAL CERTIFICATE SECONDARY EDUCATION CHEMISTRY TEACHERS

Pasheena A/P Ramathas

^aUniversity of Science Malaysia

**Corresponding author: pashee89@yahoo.com*

Abstract

Differentiated Instruction (DI) is a strategy that caters to the needs of students with varying levels of ability that has attracted the attention of many educators. Chemistry teachers inevitably face the challenge of serving academically diverse students, such as gifted and underachieving students, in regular classroom settings; hence, chemistry teachers implementing DI is significant. Differentiated instruction makes it possible to use approaches that are specific to each student's content, methodology, and resources by chemistry teachers. Green chemistry, which is an environmentally responsible and benign way of teaching and learning chemistry, is gaining importance in contemporary chemistry education. It allows students to learn the chemistry concepts while simultaneously understanding the sustainable issues inherent to them. Chemistry teachers can redirect the practical lessons to examine chemical topics from a green perspective for students. Different laboratory activities, such as comparing conventional synthesis techniques with more ecologically friendly ones or working on group projects that look into how chemical processes affect the environment, are some examples of suggested process differentiation. This method increases the effectiveness and inclusivity of addressing the International General Certificate Secondary Education (IGCSE) Chemistry curriculum's context and application focus.

Keywords: Differentiated Instruction, Green Chemistry, IGCSE Chemistry teacher

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STRENGTHENING CHEMICAL SECURITY: FROM POLICY TO PRACTICE

Christine M. Straut Langlinais,

Sandia National Laboratories, Albuquerque, NM, U.S.A

Corresponding author: cmstrau@sandia.gov

Abstract

The increasing complexity of global supply chains and the rising threats associated with chemical substances necessitate a robust approach to chemical security. Effective chemical security begins with a solid policy foundation, encompassing national regulations, international agreements, and industry standards. However, the real challenge lies in translating these policies into actionable practices that can mitigate risks associated with chemical production, storage, and transportation. This presentation will explore the critical intersection of policy and practice in strengthening chemical security, emphasizing the need for a comprehensive approach that encompasses regulatory frameworks, industry collaboration, and community engagement.

From policy to procedures, this presentation will highlight key strategies for bridging the gap, including the development of comprehensive risk assessment frameworks, the adoption of advanced technologies for monitoring and detection, and the establishment of clear communication channels among stakeholders. Success stories will illustrate effective implementations of chemical security practices across various sectors, highlighting the importance of collaboration between government agencies, industry leaders, and local communities. By fostering a culture of security awareness and preparedness, organizations can enhance their resilience against potential threats.

In summary, strengthening chemical security requires a concerted effort to ensure that policies are effectively translated into practice. This presentation aims to inspire stakeholders to take proactive steps toward enhancing chemical security, ultimately contributing to a safer and more secure future.

Keywords: Chemical Security, Risk Assessment Framework, Policy and practice, Stakeholder Collaboration

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APPLYING PRODUCT STEWARDSHIP FOR CHEMICAL SECURITY

Muhammad Anas Danial Ismail^{a,*}

^a*Henkel (Malaysia) Sdn Bhd, Chemical Industries Council of Malaysia*

^{*}*Corresponding author: anas.danial@henkel.com*

Abstract

Product stewardship has been long incorporated as an approach within chemical safety to manage a chemical product's impact on human health & safety and the environment, such as its adoption as a code of management practice in Responsible Care¹. Within the context of chemical security, however, the United States Cyber Security & Infrastructure Security Agency (CISA) defined product stewardship as a product-centered approach to the protection of dangerous materials, extending to chemicals of concern, so that manufacturers, distributors, retailers, and consumers share responsibility for reducing the potential for theft, contamination, or misuse of such chemicals for nefarious purposes². Herein, the discussion will explore how product stewardship principle is applied for chemical security purposes across a product life cycle. Best practices within the chemical industry i.e. chemical substance identification, product handling, inventory management, know-your-customer (KYC) program, will be shared to demonstrate the application of product stewardship throughout these stages.

Keywords: product stewardship, chemical security, product life cycle, dangerous materials, chemicals of concern

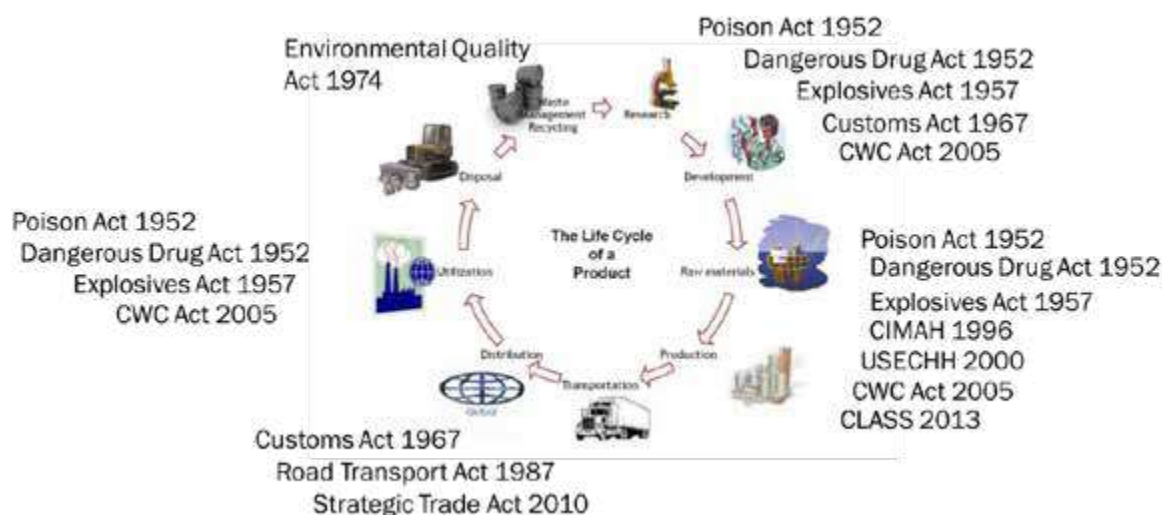


Figure 1: Legislations in Malaysia across a product lifecycle with chemical security concerns.

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EMPOWERING INSTITUTIONS: FREELY AVAILABLE TOOLS FOR CHEMICAL RISK ASSESSMENTS AND SECURITY MANAGEMENT

Maurice Payne, Christine M. Straut Langlinais

Sandia National Laboratories, Albuquerque, NM, U.S.A

Corresponding authors: maupayn@sandia.gov, cmstrau@sandia.gov

Abstract

Laboratories and research institutions often manage hundreds or thousands of chemicals, each presenting different levels of risk. Chemical safety management focuses on preventing accidental releases of hazardous materials, while chemical security emphasizes the protection, control, and accountability of these chemicals. In essence, chemical safety protects people from chemicals, whereas chemical security protects chemicals from people. Although the processes for assessing safety and security risks are similar, the associated hazards, threats, and controls are distinct. Given the limited resources for managing security risks at many institutions, it is crucial to systematically prioritize these risks to optimize resource allocation for safety improvements.

For over a decade, the Global Chemical and Biological Security (GCBS) team at Sandia National Laboratories (SNL) has developed user-friendly, freely available tools to enhance chemical risk management for resource-limited institutions. This presentation reviews these tools, highlighting their background, advantages, and limitations. The resources include: 1) three downloadable applications that provide an effective chemical inventory management system with a focus on security^{1,2}; 2) a guidebook offering a step-by-step approach to conducting chemical risk assessments for academic institutions³; 3) three physical security applications designed for performing chemical security vulnerability assessments at facilities; and 4) reference documentation outlining best practices for small-to-medium chemical facilities and the transportation of hazardous materials.

These tools empower institutions to enhance their chemical risk management practices. By systematically prioritizing safety and security risks, these initiatives protect personnel and the environment while fostering a culture of safety and accountability in chemical handling. Ultimately, this work contributes to promoting safer laboratory environments and mitigating potential hazards associated with chemical use in research settings.

Keywords: Chemical Risk Management, Risk Assessment, Inventory Management

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GLOBAL STANDARDS IN CHEMICAL WARFARE AGENT ANALYSIS: INSIGHTS FROM OPCW DESIGNATED LABORATORIES

Jakub M. Milczarek^a, Daniel Noort^{a*}

^a *Organisation for the Prohibition of Chemical Weapons, The Hague, The Netherlands*

^{*} *Corresponding author: daniel.noort@opcw.org*

Abstract

The Organisation for the Prohibition of Chemical Weapons (OPCW) is the implementing body for the Chemical Weapons Convention (CWC) ¹, which entered into force on 29 April 1997. The OPCW, with its 193 Member States, oversees the global endeavour to permanently and verifiably eliminate chemical weapons.

The CWC includes verification regime for the compliance of Member States with the Convention. One of the verification tools utilised by the OPCW Inspectors is on-site analysis by use of mobile laboratory. In case there is a need for the off-site verification, the OPCW relies on assistance of so-called Designated Laboratories (DLs) network established and maintained through Proficiency Test (PT) programs organised by the OPCW Laboratory.

The OPCW verification regime targets chemicals listed in three schedules of the CWC Annex of Chemicals, covering lethal agents, e.g. nerve agents, choking agents, blood agents, blister agents etc. and their major precursors. The PT programs comprise of screening of those chemicals in environmental samples (e.g. soil, water, drain, wipes etc.) and biomedical samples (plasma, urine, tissue etc.). The target analytes of environmental samples are intact agents and degradation products, while the target analytes of biomedical are biomarkers formed after exposure to toxic chemicals listed in CWC. In addition to already established Environmental PT and Biomedical PT programs, a third Biotoxin PT program, focused on the two CWC-scheduled biotoxins, i.e. saxitoxin and ricin is currently in a trial phase.

One of the tools developed at OPCW for use both during the on-site inspections and by DLs is the OPCW Central Analytical Database (OCAD) which contains analytical data for scheduled and some non-scheduled chemicals relevant to CWC. The OCAD containing IR, MS, NMR, GC(RI), MS/MS and GC-HRMS data is updated annually and shared with all Member States in form of DVD, USB stick or a download link.

Keywords: Chemical Weapons, Chemical Weapons Convention, Proficiency Test, Designated Laboratory, OPCW Central Analytical Database

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RECENT ADVANCEMENTS IN CHEMICAL SAFETY PROTOCOLS IN TUNISIA

Ghayth Rigane*

University of Kairouan, Peripheric Road Dar ElAman, 3100, Tunisia.

*Corresponding author: gaith.rigan@yahoo.fr

Abstract

Chemical safety is a critical aspect of sustainable industrial development and public health protection. This study highlights recent advancements in chemical safety protocols implemented in Tunisia, reflecting the nation's commitment to minimizing risks associated with chemical use, storage, and disposal. The study outlines updates to national regulations and their alignment with international frameworks such as the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). Key achievements include the introduction of improved risk assessment methodologies, enhanced training programs for industrial operators, and stricter monitoring mechanisms. Case studies from various sectors showcase successful applications of these protocols and their impact on reducing environmental and health hazards. Challenges such as resource constraints and compliance enforcement are also discussed, alongside proposed solutions. These advancements represent a significant step toward achieving safer industrial practices and sustainable development.

Keywords: Chemical Safety, Sustainable Development, Risk Management, Regulatory Compliance, Tunisia



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ENHANCING LABORATORY SAFETY AND SECURITY EDUCATION IN SALAHADDIN UNIVERSITY-IRAQ WITH 3D ANIMATION AND VIRTUAL REALITY: A NEW APPROACH FOR IMPROVING STUDENT ENGAGEMENT AND AWARENESS

Sangar S. Ahmed *, Media Noori, Hunar Yasin Muhammad

Department of Chemistry, College of Science, Salahaddin University-Erbil, Erbil, Kurdistan Region, Iraq.

**Corresponding author: sangar.ahmad1@su.edu.krd*

Abstract

Laboratory safety and security education in Kurdistan Region Government (KRG) universities and institutions predominantly follow a classroom-based approach, where students are passive recipients of information, either reading extensive textual materials or listening to instructors. This kind of learning model can lead to reduced attention and motivation, diminishing the effectiveness of the safety and security course.¹ Additionally, laboratory safety curricula often overlook practical applications and comprehensive evaluation methods and fail to engage students' interests.²⁻³ As a result, the overall impact of safety education is limited, leaving students inadequately prepared to manage real-world laboratory risks.⁴

This study aims to improve laboratory safety education by incorporating 3D animations, virtual reality (VR), and engaging narration to reinforce safety messages, raise awareness, and encourage safe practices among students in science laboratories. Thirty students from the first stage from the Chemistry Department at Salahaddin University participated in the study, divided into two groups, each receiving a different form of laboratory safety education. Upon completing the safety training, students took a safety exam on a dedicated testing platform. The results were then analysed to evaluate the effectiveness of the different educational approaches.

The findings indicate that laboratory safety and security education incorporating 3D animation and virtual reality (VR) technologies is a focused, cost-effective, and user-friendly approach that notably improves students' understanding of safety protocols. This method effectively addresses the limitations of the traditional safety and security model, which often lacks hands-on practice, by enhancing student engagement and elevating the overall quality of safety education. Consequently, 3D animation and VR technologies present an innovative and impactful solution for laboratory safety and security instruction, playing a pivotal role in supplementary teaching and promoting safer laboratory environments.

Keywords: laboratory safety, 3D animations, virtual reality, Awareness

ENHANCING COMPLIANCE TO PROMOTE A CULTURE OF SAFETY IN A PHILIPPINE RESEARCH INSTITUTE

Jonah Bondoc^{a,*}, Maria Auxilia Siringan^a, Ladylaine Sientel Estamo^a, Charita Kwan^a

*^aNatural Sciences Research Institute (NSRI), University of the Philippines (UP),
Quezon City, Philippines.*

**Corresponding author: jlbondoc@up.edu.ph*

Abstract

The Natural Sciences Research Institute (NSRI) of the University of the Philippines-Diliman (UPD) has four (4) in-house laboratories that render various types of technical services and conduct research activities that generate hazardous wastes. To ensure regulatory compliance and commitment to environmental responsibility and employee safety, the NSRI Safety and Security Committee (NSRI-SSC) was established in 1995. Subsequently, a Chemical Waste Management System project was initiated in 1997. It aimed to develop methods for the treatment and disposal of chemical wastes in accordance with national regulations. This project has now evolved as the NSRI Chemical Safety and Chemical Waste Management Program (NSRI-CSCWMP). This paper presents the program's core components that include: (1) strict adherence to the policies set forth by the Department of Environment and Natural Resources (DENR) of the Philippines, Philippine National Police, Philippine Drug Enforcement Agency, and the Philippine Professional Regulation Commission, (2) appointment of a DENR-accredited Pollution Control Officer - Chemist, (3) protocols for the procurement, handling, labeling, and storage of chemicals, and (4) segregation of hazardous wastes and their annual hauling by a government-registered third-party transporter and treater. Furthermore, the program has an active chemical exchange scheme to minimize waste generation. Moreover, the long-standing policy of the NSRI-SSC on the conduct of the biannual safety and security seminars to all new personnel has been continually implemented to foster awareness on the Good Laboratory Practice, proper use of safety equipment, including personal protective equipment, emergency response, among others. These integrated safety frameworks ensure that NSRI upholds its responsibility to the environment and public health, making the NSRI-CSCWMP a model to other research institutions both within the University and beyond.

Keywords: chemical safety, hazardous waste management, pollution control officer, Good Laboratory Practice, personnel safety training

ENHANCING CHEMICAL SECURITY WITH COMPREHENSIVE SECURITY MEASURES FOR CHEMICAL LABORATORIES AND STORAGE FACILITIES - UNIVERSITY OF SULAIMANI, KURDISTAN REGION-IRAQ

Diary I.Tofiq^{a,b,*}, Hemin H. Roghzai^a, Hanar Q. Hassan^a, Rebaz F. Hamarawf^a, Nian N. Mohammad^a, Shakhawan A. Mhamad^c, Rebwar S.Mohammad^c

^a *Chemistry Department, College of Science, University of Sulaimani, Kurdistan Region Iraq*

^b *Safety Training Center, Research and Development Center, University of Sulaimani, KR-Iraq*

^c *Chemistry Department, College of Education, University of Sulaimani, Kurdistan Region Iraq*

**Corresponding author: diary.tofiq@univsul.edu.iq*

Abstract

To improve chemical security at academic institutions, it's crucial to have secure storage and a reliable inventory system. Secure storage reduces incidents and unauthorized access. Enhanced security measures and barriers to sensitive areas reinforce the institution's security infrastructure. Our initiative started with forming teams across nine colleges at Sulaimani University that have chemicals in their laboratories and storage facilities. They conducted inspection and assessed safety and security risks in chemical warehouses then reported their findings to the university's leadership. Depending on the assessment results we focused on the most hazardous storage areas, at the college of science and the college of education. These two colleges have substantial chemistry departments with many students and extensive chemical usage and stored chemicals. To prevent the accumulation of large amounts of materials in storage, all other colleges were informed about the types and quantities of chemicals to be replaced as needed and were kept informed about the available materials. Furthermore, the teams compiled a list of unlabelled and expired substances in storage, which was forwarded to the chemical security office for further action.

Maintaining a well-structured inventory system in chemical storage ensures precise chemical tracking, accurate record-keeping, and monitoring of chemical quantities. This system facilitates efficient application and collection of chemicals and helps quickly identify any discrepancies or missing items in both Chemical storages. Upon completing our efforts, we successfully enhanced the security of the chemistry departments, storage areas by providing them with the required security equipment. Specific improvements include: Installed surveillance camera (CCTV) to monitor all hazardous areas and entry points, Installing the emergency door and upgraded the treasury doors to standard doors featured with access control, magnetic lock, and figure print door lock to regulate the movement of materials according to standards and control access to the treasury buildings. Collectively, these measures ensure a safe and secure environment for all employees and the community.

Keywords: Chemical Security, Chemical storage, Security measure, Risk assessment, inventory system.

CHEMICAL SAFETY AND SECURITY COMPLIANCE OF SELECTED HIGHER EDUCATION INSTITUTIONS IN THE PHILIPPINES

Gideon A. Legaspi^{a,*}

*Physical Sciences Department, College of Science
De La Salle University-Dasmariñas
City of Dasmariñas, Cavite, Philippines 4115
Corresponding author: galegaspi@dlsud.edu.ph

Abstract

A comprehensive survey on chemical safety and security compliance of selected higher education institutions (HEIs) in the Philippines was carried out using a survey tool with a 5-point Likert scale. Purposive sampling was done, and a total of 62 respondents out of 80 (77.5%) participants have volunteered to answer the survey. Around 63% of the respondents are from private HEIs, while the rest are from public HEIs. About 39% of the respondents are from Luzon, 37% from Visayas, and 24% from Mindanao. For chemical security compliance, the mean compliance rating is 3.70 (moderate level of compliance). The most strongly complied chemical security measures are the purchase of chemicals from licensed vendors (4.24), the restriction on taking chemicals out from the laboratory complex (4.16), and the prohibition of outsiders in the laboratory unless duly authorized (4.11). Meanwhile, the least complied measures are the secure storage of flammable chemicals (2.98), chemical purchasing security protocols (3.05), and the secure storage of acids (3.10). For chemical safety compliance, the mean compliance rating is 3.48 (moderate level of compliance). The most strongly complied chemical safety measures are the provision of adequate fire extinguishers (4.05), the posting of safety guidelines in each laboratory room (3.89), and the monitoring of the laboratory safety compliance of the students (3.89). Meanwhile, the least complied measures are the provision of adequate fire blankets (2.44), the provision of adequate chemical spill kits (2.66), and the provision of an updated chemical laboratory safety manual (3.06). The participants have identified several difficulties that hinder their compliance with the lack of financial means and support (87%), lack of adequate laboratory personnel (70%), and lack of sufficient training (67%) as the top three reasons. Appropriate recommendations were suggested to strengthen institutional compliance and foster a stronger chemical security and safety culture.

Keywords: chemical safety, chemical security, safety culture, security culture, chemical education

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STRENGTHENING CHEMICAL SAFETY AND SECURITY MANAGEMENT IN MALAYSIA: THE CAPABILITY OF THE DEPARTMENT OF CHEMISTRY MALAYSIA.

Azharuddin Abd Aziz^{a*},

^a*Department of Chemistry Malaysia, Jalan Sultan, 46661 Petaling Jaya, Selangor, Malaysia*

^{*}*Corresponding author: azharuddin@kimia.gov.my*

Abstract

The Department of Chemistry Malaysia (KIMIA Malaysia) plays a critical role in protecting, maintaining and improving quality of life through scientific laboratory services and solutions. Its responsibilities also extend to chemical safety and security aspect, with a focus on regulating industrial chemicals, chemical warfare agents, and dual-use chemicals. Operating through a network of 14 accredited laboratories, KIMIA Malaysia delivers scientific analysis, forensic expertise, and enforcement support to uphold national and international regulations. Additionally, it strengthens chemical security measures with specialized CBRNe response teams and mobile laboratories, facilitating real-time detection and assessment of chemical threats.

KIMIA Malaysia also able to supports policy options in chemical security management, including technology-driven monitoring, identifying emerging threats, standardizing databases, and strengthening inter-agency coordination. The department support enforces regulations such as Environmental Quality Act and Hazardous Waste Regulations, the Strategic Trade Act 2010 and the Chemical Weapons Convention Act 2005, underscores the importance of chemical safety and security, addressing both health hazards and the potential for chemical misuse. By collaborating with law enforcement, customs, environmental and health agencies, KIMIA Malaysia mitigates risks associated with chemical terrorism, industrial hazards, and illegal chemical trade.

Through international cooperation and legislative support, KIMIA Malaysia capable to strengthens Malaysia's chemical governance framework, ensuring a secure and well-regulated chemical environment. Its expertise in analyzing toxic chemicals, verifying compliance, and supporting emergency response efforts reinforces Malaysia's position as a leader in chemical safety and security management.

Keywords: Chemical safety, chemical security, industrial chemicals, dual-use chemicals, policy enforcement.

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AN APPLICATION OF CONTEMPLATIVE EDUCATION FOR PROMOTING SAFETY CULTURE IN CHEMICAL LABORATORIES

Wisa Supanpaiboon*

Department of Biochemistry, Faculty of Medical Science, Naresuan University

Head of Naresuan University Chemical Safety Committee

**Corresponding author: supanpaiboon@gmail.com*

Abstract

Laboratories are workplaces that are subject to both accident and chronic disease risks. The National Research Council of Thailand (NRCT) has prominently promoted safety standards since 2017, which set guidelines and regulations for chemical laboratory safety practices to protect workers from hazards in research environments. Laboratory safety standards, NRCT peer evaluation and TIS 2677-2558, were introduced for chemical laboratories. General training courses are designed to provide only “technical skills or knowledge” from the process or learning format that is packed with information or content. Contemplation is a teaching method that can promote soft skills and encourage laboratory users to develop self-understanding, critical thinking, and social skills.

Naresuan University has developed a curriculum for laboratory safety training that applied contemplative education for the cognitive learning process to enhance safety practices and create a sustainable safety culture integrated with technical safety skills in three steps. The first step was to create an atmosphere of trust that allowed the participants to feel free and secure to communicate in the class. The potential consequences of injury and illness from laboratory hazards including the losses of a loved one and productivity were discussed using case studies and role plays as the second step and followed by technical skills such as chemical toxicity or safety measures to meet the content requirements.

The training activities focused on learning participation to develop safety awareness through various activities including deep listening, mindfulness meditation, reflection, esthetic conversation, volunteer activities, art and music as well as through scenarios and role plays. The training process also allowed the participants to discuss and reflect on the value of lessons learned, resulting in attitude changes by having empathy and showing compassion as well as environmental concern.

Keywords: contemplative education, safety culture, laboratory safety standard, soft skills

ENHANCING FUME HOOD SAFETY WITH AUTOMATED LOCAL EXHAUST VENTILATION (LEV) SENSORS: A CASE STUDY AT THE DEPARTMENT OF CHEMISTRY, MALAYSIA HEADQUARTERS

**Ts. Dr. ChM. Aidil Fahmi Shadan*, ChM. Muhammad Fazli Mad Saad,
ChM. Muhammad Haniff M. Zahari, and Mr. Muhammad Hafiz Abd Rahman**

OSH Section, Department of Chemistry, Malaysia Headquarters

**Corresponding author: aidilfahmi@kimia.gov.my*

Abstract

Fume hoods are essential for ensuring safe chemical handling in laboratories. However, their effectiveness largely depends on the consistent and accurate monitoring of airflow. Traditional manual methods, such as using anemometers, while widely accepted, present significant challenges. These include a reliance on human intervention, time-intensive processes, and the potential for inconsistent readings. Such limitations can result in undetected airflow irregularities, increasing the risk of exposure to hazardous substances and compromising safety compliance. To address these challenges, the Department of Chemistry, Malaysia Headquarters, implemented an automated Local Exhaust Ventilation (LEV) sensor system across 43 fume hoods. This system enables real-time airflow monitoring, ensuring immediate detection of anomalies and reducing the need for manual testing. This study evaluates the performance of the automated LEV system by comparing sensor data with manual anemometer readings. The results demonstrate the system's accuracy, reliability, and ability to detect airflow inconsistencies promptly. Key operational benefits include reduced maintenance time, improved safety compliance, and enhanced user satisfaction. By overcoming the limitations of traditional methods, this initiative highlights the potential of automation in strengthening safety measures in laboratory settings. It serves as a model for integrating innovative technologies in chemical risk management, fostering safer and more efficient laboratory environments.

Keywords: Local Exhaust Ventilation, Fume Hood, Chemical Laboratory, Automation, Safety Monitoring

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COUNTERING DIVERSION OF PHARMACEUTICAL BASED AGENTS OR COMPOUNDS ALONG THE CHEMICAL SUPPLY CHAIN FOR THE IMPROVEMENT OF CHEMICAL SECURITY

Abul Basher Miah

Ex-President and Present Treasurer of Bangladesh Chemical Society

**Corresponding author: abmiah71@gmail.com*

Abstract

The weaponization risk and security threats associated with the procurement of weaponizable pharmaceutical compounds along the lawful supply chain is a known phenomenon. Countering the diversion of pharmaceutical-based agents or compounds along the chemical supply chain is a great concern nowadays, as it challenges chemical security best practices in the pharmaceutical sector. To ensure this, we first have to identify the most suitable practices to increase supply chain security and customer vetting in the pharmaceutical industry to strengthen the security of procurement of weaponizable pharmaceutical compounds. Then, we should analyze chemical security approaches and the best possible countermeasures to prevent State-based proliferation of weaponizable pharmaceutical compounds.

With this view in end, Global trend as well as Bangladesh's production of pharmaceuticals and export market should be discussed and highlighted. The legitimate uses of pharmaceuticals and chemicals in pharmaceuticals application including in health and medicine will be discussed. In this context it would be worthily to mention here that the multinational chemical companies (MNCC) are playing an important role of the Global Pharmaceutical supply chain. Does code of conduct and ethics can change the behavior of MNCC? The growing threats of pharmaceutical based agents will also be highlighted. Some examples of pharmaceuticals supply chain threats and challenges around the globe should be discussed. The role of diplomatic success and international organizations like the "Organization for the Prohibition of Chemical weapons" (OPCW) will be discussed. How supply chain security in the pharmaceutical sector can be improved will also be highlighted. The specific roles of Government ministries, industries, academia will be discussed. Customer vetting is also important to ensure supply chain security. So, how this can be introduced meaningfully will be discussed. Then Know your customer, access and security control and potential red flags for illicit procurement will be discussed. Chemical security maturity models are also relevant, and will be the focused.

In fine, effectiveness of countermeasures for diversion of pharmaceuticals-based compounds /agents along the chemical supply chain will be recollect further for ensuring chemical security best practices.

Keywords: weaponizable pharmaceutical compounds, diversion of pharmaceutical-based agents or compounds, supply chain security and customer vetting, countermeasures to prevent State-based proliferation, know your customer and chemical security maturity models.

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ENHANCING CHEMICAL SAFETY IN THAILAND: INCIDENT ANALYSIS AND KEY LESSON FOR INDUSTRIAL PRACTICES

Ong-art Thanetnit^a, Supawan Tantayanon^{b,*}

^a *Center for Safety, Health and Environment, Chulalongkorn University.*

^b *Chemistry Department, Faculty of Science, Chulalongkorn University.*

**Corresponding author: Supawan.t@chula.ac.th*

Abstract

Chemical safety is a critical priority for industrial operations, influencing human health, environmental protection, and business stability¹⁻². This study analyzes 30 chemical incidents reported over the past decade at workshops organized by the Council of Science and Technology Professionals (CSTP) in Thailand. These workshops, which involved participants from diverse sectors, provided insights into significant chemical accidents within their respective industries. Incidents were categorized by company profiles, accident types, root causes, locations, hazardous chemicals involved, and contributing factors. Key findings reveal that 60% of the incidents were major accidents, with human error responsible for 77% of cases and operational failures accounting for 50% of the root causes. Laboratories were the most frequent site of incidents (50%), and chemical releases and exposures each accounted for 33% of incident types. Corrosive and toxic chemicals were the most commonly involved substances. These findings highlight the urgent need for enhanced chemical safety training and improved operational protocols to mitigate risks and strengthen safety practices across chemical industry in Thailand

Keywords: chemical safety, industrial incidents, operational safety, hazard prevention

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IMPLEMENTATION STATUS OF CHEMICAL SAFETY AND SECURITY MANAGEMENT (CSSM) IN MALAYSIA BASED ON OPCW INDICATIVE GUIDELINES

Hazlina Yon^{a,*}, Rizwana Rusle^b,

^{a,b} *Department Of Occupational Safety and Health Malaysia,*

**Corresponding author: *hazlina@mohr.gov.my, rizwana@mohr.gov.my*

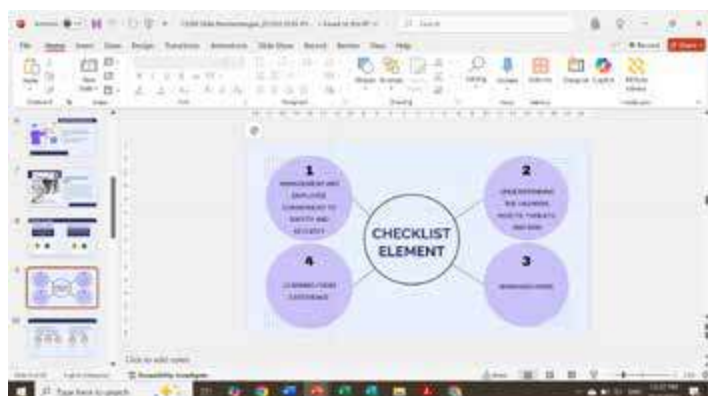
Abstract

OPCW introduced Indicative Guidelines for Chemical Safety and Security in Small and Medium-sized Enterprises to Foster the Peaceful Uses of Chemistry in 2021. This guideline has been adopted by Malaysia to develop a simple checklist to be used by industries to promote good management of chemical safety and security. Malaysia commemorated this through an event launched by the Director Deputy General of the Department of Occupational Safety and Health (DOSH) Malaysia on the 23rd of October 2024 in Putrajaya. It is organized by the Chemical Management Division of the DOSH.

The main aim of the adopted checklist is to foster best practices in chemical safety and security and promote peaceful uses of chemistry. In developing the checklist, we benchmarked with various sectors of industries from oil and gas industries, chemical manufacturers and many others. Engagement involves multiple workshops, pilot tests, and the final launch in October 2024. The checklist includes management commitment, understanding hazards, managing risks, and learning from experience. The weightage is 30% for management commitment, 30% for understanding hazards, 20% for managing risks, and 20% for learning from experience.

Through the process of adopting the checklist, we found the following: Low Compliance on Security-Related topics where nearly 50% of workplaces failed to reach Level 4 (*Fully Implemented*) and low compliance of understanding of Hazards and Risks. Challenges found where many workplaces were unaware of dual-use equipment, which can be used for both beneficial and harmful purposes and chemical safety management was easier to comply with, while chemical security management was more challenging.

Keywords: chemical safety, chemical security, OPCW Indicative Guidelines, checklist, CSSM.



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CHEMICAL SAFETY AND SECURITY REGULATORY COMPLIANCE IN INDONESIA

Ikawati Suryani^a

^a*Responsible Care Indonesia*

**Corresponding author: ikasuryani139@gmail.com*

Abstract

The chemical safety and security regulatory compliance is not an easy topic as Indonesia regulatory frameworks is little bit overlapping and or sometimes confusing, because there are so many chemical related regulations in place. Through this topic, it gives the snapshot of the most relevant regulations to the workshop participants including its compliance. This topic aims to raise the awareness of chemical safety and security regulations to strengthen supply chain chemical safety and security measures. As well as to enhance chemical safety and security regulatory awareness for importers, distributors, traders, including informal markets and its compliance requirements in Indonesia. This topic is equipping importers/traders in both formal and informal markets with the essential knowledge and skills to enhance chemical safety and security awareness to strengthened partnership and cooperation among the relevant stakeholders. To get a better understanding on the whole picture of Indonesia regulatory compliance, it is started with the quick snapshot on the chemical industry in Indonesia. Then it will go further on the big picture of Indonesia Regulatory Framework such as the Hierarchy of Indonesia Regulation and the diagram of Indonesia Chemical Regulatory Frameworks based on the applications, chemical composition, government agencies, regulations, and its legal requirements. The deep dive Indonesia Chemical Regulations will be shared in snapshot table and in more detail information, such as the owner of regulations, the scope, the regulatory requirements, the link of relevant regulations etc. It is not only covering the existing/ updated regulations for Chemical Import and Distribution of Chemicals, but also for the drafted regulations.

Keywords: Regulatory Compliance, Chemical Safety and Security, Indonesia Regulatory Framework

LESSON LEARNT FOR CHEMICAL SECURITY IN VIETNAM

Nguyen Bui, PhD Nguyen Xuan Sinh

Vietnam Responsible Care Council

**Corresponding author: buiducnguyen10@gmail.com*

Abstract

The increasing misuse of Dual Use Chemical Weapon Agents & Precursors in Vietnam - ranging from deliberate poisoning cases and illegal production of narcotics - has raised concerns about public security and health. These incidents highlight critical gaps in the control of dual-use chemicals, and precursors, which have been exploited due to inadequate oversight from private sectors.

We have been studying key lessons learned from recent cases in Vietnam, emphasizing the root causes behind chemical security failures along the supply chain. It will also propose appropriate measures, including enhanced cross-sector collaboration, and capacity-building initiatives for both industries and enforcement agencies. Strengthening chemical security is not just a regulatory necessity but a fundamental safeguard for protecting communities and ensuring sustainable development. Herein discussion will be focused on the following points with the goal of strengthening chemical security

1. Chemical supply chain security challenges.
2. The Role of Authorities and Private Sectors.
3. Recommendations for sufficient Chemical Security Management.

Keywords: chemical security, dual use chemical, protecting community

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HEALTH, SAFETY AND ENVIRONMENTAL RISK ASSESSMENT OF CHEMISTRY LABORATORIES IN HIGHER EDUCATIONAL INSTITUTIONS IN LAGOS, NIGERIA

Popoola Oluseun^{*a}, Ayilara Deborah^a, Olayiwola Basirat^a,

^a*Yaba College of Technology, Lagos, Nigeria*

**Corresponding author: oluseun.popoola@yabatech.edu.ng*

Abstract

Chemical laboratories in higher education institutions (HEIs) play a crucial role in education and research. The availability of chemicals of concern and other factors present significant health, safety, and environmental (HSE) risks. This study is aimed at the risk assessment of chemical laboratories in the selected HEIs in Lagos, Nigeria using primary data (structured questionnaires), secondary data (observation checklists for chemical laboratories) and a combination of the above tools to compute the potential risks¹. Risks associated with concentrated acid digestion were also determined. The findings generally show satisfactory conditions, with 84% of laboratories being well-ventilated. However, critical gaps indicated that 24% lacked emergency response plans, 34% did not have Safety Data Sheets readily available, 23% reported poor waste disposal practices and lacked updated chemical inventory. Risk assessments identified severe hazards, including ethanol (safety risk score of 25) and sodium hydroxide (health risk score of 25), both classified as very high risk, while the heavy metal digestion process using concentrated acids (score of 25). Compliance levels varied, with universities at 85%, colleges of education at 69%, while polytechnics gave 54%. The study indicated the need for improved training, particularly for students representing 85% of the respondents, as well as better waste management and ventilation systems². The study underscores the need for targeted interventions to enhance safety protocols and create safer, more sustainable chemical laboratory environment.

Keywords: Health, Safety, Environmental Hazards, Risk Assessment, Chemical Laboratories, Higher Education

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ENHANCING CHEMICAL SECURITY INFRASTRUCTURE AT BENUE STATE UNIVERSITY, MAKURDI, NIGERIA

Linus Aposu

Institute of Chartered Chemists of Nigeria, Abuja, Nigeria

laposu@yahoo.com

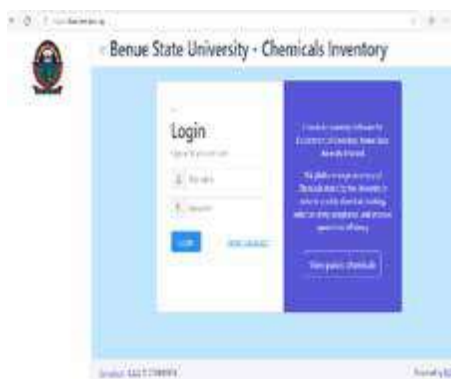
Abstract

The project was designed, developed and implemented to improve the chemical security infrastructure in chemistry complexes comprising six laboratories and two major chemical storage facilities at Benue State University, Makurdi, Nigeria, to ensure the safe storage and handling of hazardous materials. A thorough risk and vulnerability assessment conducted before the project revealed deficiencies, including inadequate access controls, insufficient chemical storage facilities, and a lack of surveillance systems.

To address these issues, the project implemented robust security measures such as secure chemical storage cabinets, electronic access control systems, surveillance systems, and an advanced inventory management system. These enhancements effectively mitigate unauthorized access, theft, and chemical misuse risks. Furthermore, training sessions equipped laboratory personnel with best practices in chemical security and emergency response, fostering a culture of responsibility and compliance.

This initiative, supported by the Benue State University Management and the CRDF Global Chemical Security Improvement Grant, has fortified the university's chemical security infrastructure and created a replicable model for academic institutions across the region. These efforts contribute significantly to local and global goals of promoting chemical safety and security while ensuring sustainable use of chemical resources in education and research.

Keywords: Chemical Security; Infrastructure; Hazardous Materials; Surveillance Systems; Sustainability



EMPOWERING COMMUNITIES: ADVANCING CHEMICAL SAFETY AND SECURITY THROUGH INNOVATION AND EDUCATION

Ridha Ben Salem*

Organic Chemistry Laboratory LR17ES08, Sciences of Sfax Faculty, Chemistry Department, B.P « 1171 » 3038, University of Sfax, Tunisia.

**Corresponding author: ridhabensalem@yahoo.fr*

Abstract

Enhancing chemical safety and security is a global imperative that requires inclusive, community-driven approaches. This paper investigates the role of innovation and education in empowering communities to effectively manage chemical risks and ensure sustainable development. Technological advancements, such as digital hazard tracking systems, artificial intelligence for risk prediction, and green chemistry solutions, provide new tools for mitigating chemical threats. Concurrently, education programs tailored to local contexts are essential for building awareness, fostering safety cultures, and equipping communities with practical skills. The study examines case studies from diverse regions, illustrating how integrative strategies that combine technology and education can address complex challenges, including industrial accidents, hazardous waste management, and chemical terrorism. The findings reveal that collaboration among governments, industries, academic institutions, and local stakeholders is critical for success. This research underscores the potential of innovation and education to empower communities, reduce vulnerabilities, and advance global chemical safety and security initiatives.

Keywords: Chemical Safety, Innovation, Security, Global Collaboration



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BIOSECURITY CONCERNS IN CHEMICAL RESEARCH: THREATS AND MITIGATION STRATEGIES

Prakash Balu*

Department of Biotechnology, Vels Institute of Science, Technology and Advanced Studies, Chennai.

**Corresponding author: prakazbt@gmail.com*

Abstract

Chemical research plays a vital role in scientific advancements, but it also presents significant biosecurity risks. Unauthorized access, dual-use research concerns, and the potential misuse of hazardous chemicals pose serious threats to public safety and environmental health¹. This presentation explores the critical biosecurity challenges in chemical research, emphasizing threats such as terrorism, accidental releases, and inadequate regulatory compliance. International frameworks, including the Chemical Weapons Convention (CWC)² and Biological and Toxin Weapons Convention (BWC), provide regulatory guidelines³, but effective implementation at institutional levels remains a challenge. Key mitigation strategies include strict access control, chemical inventory management, risk assessment protocols, and secure storage and disposal methods. Additionally, fostering a strong safety culture through training programs, security audits, and inter-agency collaboration is crucial in preventing biosecurity breaches.

Recent technological advancements, such as AI-driven threat detection, blockchain-based chemical tracking, and IoT-enabled monitoring systems⁴, offer promising solutions to enhance chemical security. Case studies of past security breaches highlight the importance of proactive measures in mitigating risks.

Strengthening global cooperation and implementing innovative security technologies are essential for minimizing biosecurity threats in chemical research⁵. This presentation aims to raise awareness among researchers, policymakers, and industry professionals about the importance of robust biosecurity frameworks. By integrating research findings with best practices, institutions can ensure a safer and more secure research environment, balancing scientific progress with responsible chemical management.

Keywords: Biosecurity, Chemical Safety, Dual-Use Research, Security Audits, AI in Biosecurity

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PUBLIC-PRIVATE PARTNERSHIPS FOR ENHANCING CHEMICAL SAFETY AND SECURITY

Sahila Chellamuthu*

Department of Commerce, SRM Institute of Science and Technology, Ramapuram Campus, Chennai - 600089

**Corresponding author: sahiladr@gmail.com*

Abstract

Chemical research plays a vital role in scientific advancements, but it also presents significant biosecurity risks. Unauthorized access, dual-use research concerns, and the potential misuse of hazardous chemicals pose serious threats to public safety and environmental health¹. This presentation explores the critical biosecurity challenges in chemical research, emphasizing threats such as terrorism, accidental releases, and inadequate regulatory compliance.

International frameworks, including the Chemical Weapons Convention (CWC)² and Biological and Toxin Weapons Convention (BWC), provide regulatory guidelines³, but effective implementation at institutional levels remains a challenge. Key mitigation strategies include strict access control, chemical inventory management, risk assessment protocols, and secure storage and disposal methods. Additionally, fostering a strong safety culture through training programs, security audits, and inter-agency collaboration is crucial in preventing biosecurity breaches.

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Keywords: Biosecurity, Chemical Safety, Dual-Use Research, Security Audits, AI in Biosecurity

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ASSESSMENT OF CHEMICAL SAFETY AND SECURITY KNOWLEDGE IN TUNISIAN ACADEMIC AND RESEARCH INSTITUTIONS: IDENTIFYING GAPS AND TRAINING NEEDS

RABTI A.,^{a*} MOUSSAOUI Y.,^b BEN SALEM R.,^c BEN ROMDHANE H.^{d*}

^a *Laboratory of Materials, Treatment, and Analysis (LMTA), National Institute of Research and Physicochemical Analysis (INRAP), Biotechpole Sidi Thabet, 2020 Sidi Thabet, Tunisia.*

^b *University of Gafsa, Faculty of Science of Gafsa, Campus Universitaire Sidi Ahmed Zarroug - 2112 Gafsa, Tunisia.*

^c *University of Sfax, Faculty of Science of Sfax, Route de la Soukra km 4 - BP 1171-3000 Sfax, Tunisia.*

^d *University of Tunis El Manar, Faculty of Science of Tunis, Farhat Hached University Campus, Tunis El Manar, 2092 Tunis, Tunisia.*

** Corresponding authors: amal.rabti@fst.utm.tn , hatem.benromdhane@fst.utm.tn*

Abstract:

Implementing effective chemical safety and security protocols challenges developing nations' academic institutions. This study assessed knowledge levels in Tunisian academic and research circles through two surveys, one addressed to 41 professionals and 42 students, and through three CRDF Global-funded training workshops (47 participants) held at Tunisian universities in three regions of the country between September and October 2024. The pre-assessment revealed significant knowledge gaps. The majority of participants reported no prior training in chemical security/safety. Furthermore, 47 participants were unable to clearly differentiate between safety and security concepts. While familiarity with hazard pictograms and personal protective equipment was moderate, understanding of safety data sheets, emergency procedures, and dual-use chemicals was limited. Only half of the professional staff rated their chemical safety knowledge as good or excellent, with fewer claiming proficiency in chemical security. The institutional infrastructure suffers from a lack of resources. Less than half of the respondents confirmed the existence of safety and security protocols. Moreover, while 18 participants reported never conducting safety drills, a mere 14 indicated that their institutions provide regular training. Similarly chemical waste management emerged as particularly problematic, with practices rated as average or ineffective and temporary storage being the predominant disposal method. Three two-day workshops held in Gafsa, Sfax, and Tunis (September-October 2024) addressed these deficiencies, covering risk analysis, accident prevention, threat assessment, and laboratory safety. Post-training evaluations indicated a marked improvement, with 76.1% of participants demonstrating "Very Good" understanding of key concepts. The findings demonstrate overwhelming support for additional training and standardized programs. What makes this difficult to achieve is funding limitations, cultural resistance, insufficient awareness, and lack of institutional support. This study offers a scalable model for developing nations highlighting the critical need for sustained efforts in safety protocol implementation, waste management improvements, and heightened awareness of dual-use chemicals.

Keywords: Chemical safety; Security protocols; Waste management; Training needs; Tunisia.

ESTABLISHING A MANAGEMENT SYSTEM FOR THE SAFETY AND SECURITY OF CHEMICAL SUBSTANCES

Belkacem BENGUELLA^{a,*}

*University of Tlemcen, Science Faculty, Chemistry Department,
Inorganic Chemistry and Environment Laboratory
B.P 119.Tlemcen Algeria*

**Corresponding author: belkacem_71@yahoo.fr*

Abstract

The implementation of a management system for the safety and security of chemical substances is very important for the protection of people's health, the environment and equipment against the risk and danger of chemical products. The policy adopted by our research laboratory is based primarily on training and raising the awareness of staff (students, doctoral students, technicians, etc.) about the safety and security of chemical products:

- A subject for second-year Master students on safety and security in the chemistry laboratory, with practical tests on the hazard categories of chemical products and the use of individual and collective protective equipment.
- Continuing training for doctoral students on the implementation of a safety culture that requires a commitment to high standards of good practice in prevention and response.
- Implementing a chemical product management system based on: an inventory and safety data sheet (CMS software), chemical product storage, chemical product waste management, control of access to chemical substances, etc.

An effective management system for the safety and security of chemical substances is a crucial part of our environmental research laboratory in order to achieve better prevention and ensure ongoing training for all employees.

In conclusion, the art of respecting this approach is to establish a safety measurement system guide developed thanks to the training carried out with the SANDIA laboratory.

Key words: safety, security, chemical substances, management system

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RESPONSIBLE CARE AND NICER GLOBE DRIVING EXCELLENCE IN CHEMICAL SAFETY AND SECURITY

Pranav Tripathi

Indian Chemical Council

Corresponding author: pranav.tripathi@iccmil.in

Abstract

The Indian Chemical Council (ICC), the apex national body representing India's chemical industry, has a legacy dating back to 1938 and a strong membership base of 500+ companies. ICC spearheads transformative initiatives like Responsible Care® (RC)¹ and Nicer Globe® (NG)² to enhance safety, security, and sustainability in the industry. Responsible Care® (RC) is a globally recognized, industry-driven initiative that proactively addresses public concerns about chemical manufacturing and usage, focusing on health, environmental stewardship, and safety.

Implementation in India

- 1991: RC introduced with six codes of practice
- 2006: RC verification process initiated
- Present: 90 companies actively practice RC and are verified, which is roughly 12% of India's Chemical Business
- 24 companies have signed the Global Charter of Responsible Care

In 2013, ICC launched Nicer Globe®, a comprehensive real-time monitoring technology platform aimed at enhancing chemical transportation safety and emergency response in India. Key facts of Nicer Globe:

- 80 user companies
- 900 logistics providers
- 100,000+ trained drivers
- 30+ emergency responder located at 15 high risk spots in the India's Chemical belt at distance of 200 km

In 2019, ICC introduced the Security Code as the seventh RC code, a pioneering step towards a preventive approach to chemical security. This initiative is supported by the Security Code Manual and Guidance Manual, offering clear implementation strategies. To strengthen execution, 25 RC auditors, including 10 Security Vulnerability Assessors, were trained, enabling risk assessments at 30+ facilities, covering Schedule 2 & 3 and dual-use chemicals. This effort has been achieved over a five-year period, from August 2019 to July 2024.

The Seven RC Codes and Nicer Globe® exemplify ICC's unwavering commitment to safety, security, and excellence, setting new industry benchmarks through innovation and proactive measures. The ICC's efforts to enhance safety and chemical security have been recognized with the prestigious 2024 OPCW-The Hague Award.

Keywords: Responsible Care; Nicer Globe; Global Charter; Training; Security Code

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TOWARD COHESIVE CHEMICAL SAFETY AND SECURITY EDUCATION IN ASEAN

Genejane M. Adarlo^a, Armando M. Guidote, Jr.^{b,c*},
Anna Carissa M. San Esteban^{b,c}, Hooi Ling Lee^d

^aHealth Sciences Program, Ateneo de Manila University, Quezon City, Philippines 1108

^bDepartment of Chemistry, Ateneo de Manila University, Quezon City, Philippines 1108

^cPhilippine Institute of Pure and Applied Chemistry (PIPAC), Quezon City, Philippines 1108

^dSchool of Chemical Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia

*Corresponding author: aguidote@ateneo.edu

Abstract

Chemicals of interest are mostly used in educational institutions, research facilities, and industries.¹ However, several of these chemicals pose inherent security risks as they can be used for legitimate and illicit purposes.^{1,2} Hence, there is a growing need for a comprehensive chemical safety and security education to equip students, chemists, chemical engineers, and other stakeholders with the knowledge and skills to prevent the misuse, theft, and diversion of such chemicals.³ Integrating chemical risk management into the undergraduate curriculum, for instance, can help students understand the properties of hazardous chemicals, the potential risks they pose, and the measures required for their safe and secure handling.⁴ A region-wide, coordinated approach to chemical safety and security education can promote the exchange of expertise, optimize resource distribution, build capacity, and strengthen regulatory compliance across countries. Despite its importance, there is limited literature on how chemical safety and security education is integrated into undergraduate curricula, particularly within the Association of Southeast Asian Nations (ASEAN) region. Hence, this mixed-methods study aims to investigate the extent, coverage, and emphasis of chemical safety and security education in chemistry-related undergraduate programs across ASEAN educational institutions. Data will be collected through an online survey of institutional representatives, supplemented by semi-structured interviews to gain deeper insights into the factors influencing national and institutional differences. In addition to the findings that chemical safety and security education vary significantly across ASEAN countries and even among institutions within the same country due to differences in enforcement of regulations, availability of resources, and provision of support, this study expects to observe an equal emphasis on chemical safety and security in these programs. The findings have important implications for policy development, curriculum design, industry practices, and overall public safety, contributing to a more cohesive approach to chemical risk management in the ASEAN region.

Keywords: Chemical Safety and Security Education, Chemical Risk Management, ASEAN

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CHLORINE AS A DUAL-USE CHEMICAL: THE ROLE OF CHEMICAL ANALYSIS IN ENHANCING CHEMICAL SECURITY

Nurhazlina Hamzah^{a,*}

^a*Chemical Preparedness Section (CWC & CBRNe), Department of Chemistry Malaysia.*

**Corresponding author: nurhazlina@kimia.gov.my*

Abstract

Chlorine is a dual-use chemical with both civil and military applications, and the Chemical Weapons Convention (CWC) prohibits its use as a chemical weapon under the general-purpose criterion (Article II). Chlorine is widely used in the water disinfection and chemical industries to produce plastics, drugs, microchips, and other products. Whereas, chlorine gas was employed as a choking agent during World War I, and in at least 89% of incidents in The Syrian Arab Republic between 2013 and 2018.¹

Chlorine is highly reactive with both organic and inorganic chemicals, resulting in chlorinated analogues of the precursor molecules. The identification of chlorine reaction products from various sources is complex and must be unequivocal to provide proof of its use. The Organisation for the Prohibition of Chemical Weapons (OPCW) Fact-Finding Mission reported chlorinated phenols as markers for “reactive chlorine” in environmental samples like concrete debris from the alleged chemical weapon use in Douma in 2018.²

This abstract explores the current methods and technologies employed to detect chlorine exposure during a chemical incident, with a focus on the laboratory approach. For environmental samples, gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS) have proven to be effective for identifying chlorine gas in air, water, soil, concrete and plants with chlorinated organic compounds as markers.³ The most useful biomarkers for chlorine exposure in biomedical analysis include tyrosine adducts, chlorohydrin, chloro-fatty-acids, chloro-fatty-aldehydes, and chloro-fatty-alcohols were analysed by chromatographic separation with mass spectrometric detection such as GC-MS and LC-MS.

The challenges faced by laboratories are discuss in ensuring preparedness, including the need for rapid detection system deployment, training, and standard procedures for diverse dual-use chemical scenarios. Finally, improving laboratory preparedness for chlorine detection after chemical incidents will promote fast, accurate decision-making in emergencies and recovery, enhance chemical security, and assist bring perpetrators to justice.

Keywords: Dual-use chemical, chlorine markers, biomarkers, chlorinated organic compounds, mass spectrometry.

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IMPLEMENTATION OF CHEMICAL SECURITY INITIATIVES IN THAILAND & ASEAN

***Sutthipas Wongsiriporn, Chalernsak Karnchanawarin,**

*^a Responsible Care Management Committee of Thailand (RCMCT),
Chemical Industry Club (CIC), The Federation of Thai Industries (FTI).*

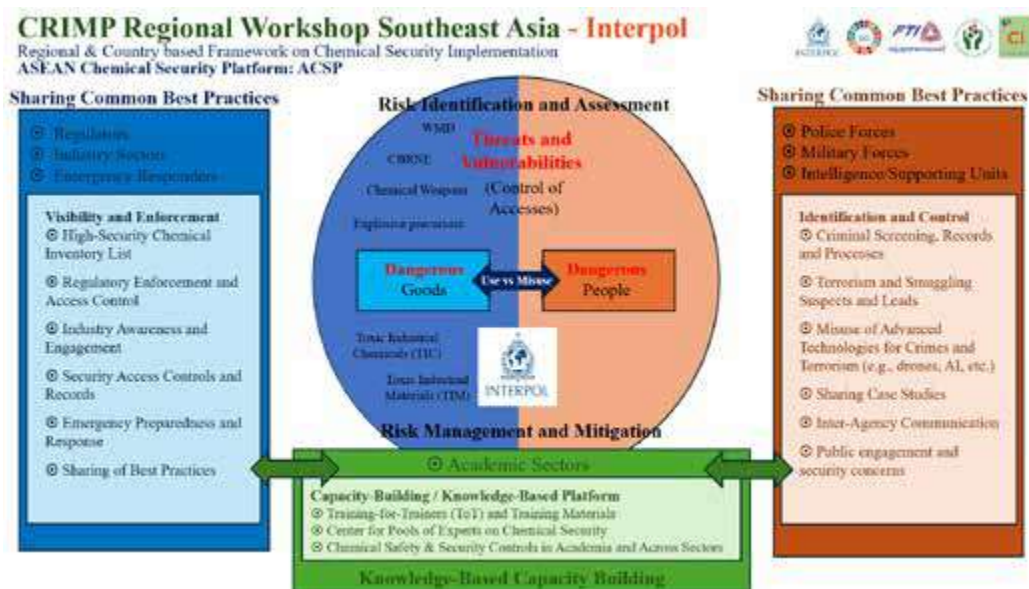
**Corresponding author: Sutthipas.wongsiriporn-1@dow.com, Toon@hazchemlogistics.com*

Abstract

RCMCT, as a leading unit for Responsible Care implementation, has initiated a collaboration with The International Criminal Police Organization (INTERPOL) to enhance chemical security in Thailand through multi-stakeholder engagement. These initiatives began with capacity-building programs under the Chemical Risk Identification and Mitigation Project (CRIMP) Workshops 1 and 2 for Thailand. This effort subsequently led to the CRIMP Regional Workshop Southeast Asia on Chemical Security which engaged four leading ASEAN member states: the Philippines, Indonesia, Malaysia, and Thailand for mutual collaboration at the regional level.

The proposed framework, based on both country-specific and regional models for chemical security, presents a challenging yet essential task for effective implementation at both levels. Therefore, the ASEAN Chemical Security Platform (ACSP) is initiated and envisioned as the pioneering program for comprehensive chemical security management in the ASEAN region.

Keywords: Chemical Security, Chemical Risk Identification and Mitigation Project, CRIMP Regional Workshop, Responsible Care Thailand, INTERPOL, ASEAN Chemical Security Platform (ACSP)



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AI MACHINE LEARNING DEVELOPMENT IN CHEMICAL SAFETY: PREDICTIVE ALGORITHMS AND PROTECTIVE MEASURES BASED ON NINE GHS SYMBOL CLASSIFICATIONS

Muhammad Aiman Hazmir ^a, Tiem Leong Yoon ^b, Hooi ling Lee ^a

a School of Chemical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

b School of Physics, Universiti Sains Malaysia, 1800 USM, Penang, Malaysia

**Corresponding author: hllee@usm.my*

Abstract

Chemical safety and security are critical aspects of industrial operations. The Globally Harmonised System (GHS) classifies chemicals into nine hazard categories, but existing classification methods rely heavily on manual evaluation, which is time-consuming and prone to human error. This study introduces a novel machine learning (ML) approach to enhance chemical hazard classification by using nine GHS symbols as target features for predictive modelling. The research objectives are: (i) To train an AI machine learning system with the use of Python in monitoring and risk analysis system, and (ii) To implement predictive modelling, data analysis, and pattern recognition for real-time hazard assessment in chemical facilities. Data was sourced from PubChem, comprising approximately 150,000 chemical entries. Preprocessing involved feature selection and data cleaning before training classification models using Python and its operating libraries such as Scikit-learn. Machine learning algorithms, including Random Forest and Support Vector Machine (SVM), were tested for performance evaluation based on accuracy, precision, recall, and F1-score. Preliminary results indicate that the ML model successfully predicts GHS classifications with good accuracy for certain classes, indicating the feasibility and potential of AI-driven risk assessment in chemical safety using the nine GHS symbols. The novelty of this research lies in its comprehensive integration of all nine GHS symbols as classification targets, which has not been extensively explored in previous studies. This study highlights the potential of AI in enhancing chemical hazard assessment, reducing dependency on experimental methods, and improving safety compliance. Future work will refine feature selection and explore deep-learning techniques for improved classification accuracy.

Keywords: Chemical Safety and Security, Machine Learning, GHS Classification, AI Risk Assessment, Python

SECURITY AND TRANSPORTATION CODES - RESPONSIBLE CARE IMPLEMENTATION IN CHEMICAL INDUSTRY

Eko Pratikto

Federation of the Indonesian Chemical Industry (FIKI)

**Corresponding author: e.pratikto@gmail.com*

Abstract

The Responsible Care initiative is a global commitment by the chemical industry to enhance environmental health, safety, and security performance throughout its operations. Central to its framework are the Security and Transportation Codes, which aim to mitigate risks associated with the handling, storage, and transportation of hazardous materials. The Security Code emphasizes measures to prevent unauthorized access, theft, sabotage, and other security threats, fostering a culture of vigilance and preparedness. It integrates physical, cyber, and personnel security practices to protect assets and mitigate risks across the supply chain. The Transportation Code ensures the safe and efficient movement of chemical products, focusing on risk assessment, route planning, and emergency preparedness. Key aspects include training personnel, engaging with stakeholders, and using advanced technologies to monitor and manage transportation operations. Implementation of these codes aligns with regulatory requirements and global standards, promoting stakeholder trust and minimizing environmental and societal impacts. By embedding these principles into their operations, organizations demonstrate their commitment to sustainability and the continuous improvement of safety, security, and operational excellence. This poster presentation explores the principles, strategies, and best practices underpinning the Security and Transportation Codes, providing insights into their critical role in the holistic implementation of Responsible Care.

Keywords: Chemical Security, Transportation Security, Responsible Care, Chemical Industry, Risks Management.

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CHEMICAL SAFETY AND SECURITY IN VIETNAM

PhD Nguyen Xuan Sinh

Vietnam Responsible Care Council.

**Corresponding author: sinhnxvinachemia@gmail.com*

Abstract

Currently, chemical security is receiving significant attention from countries around the world and international organizations focused on chemicals due to the importance of ensuring chemical security in chemical activities. Vietnam is a member of several international conventions in the field of chemicals, such as the Chemical Weapons Convention (OPCW). Recent times, Vietnam has participated in numerous international seminars on chemical security which are continuously organized, highlighting the necessity of establishing regulations on chemical security. This is crucial to prevent legal gaps that could hinder the development of laws on chemical security and ensuring that Vietnam keeps pace with international legal regulations that may be promulgated in the near future.

In 2024, The Government of Vietnam issued a Decree No. 34/2024/ND-CP regulating the implementation of the Convention on the Prohibition of the Development, Production, Stockpiling, Use and Destruction of Chemical Weapons. Currently, Vietnam is drafting a new Chemical Law to replace the 2007 Chemical Law. Currently, Vietnam is drafting a new Chemical Law to replace the 2007 Chemical Law. At the same time, regulations under the Law will be developed and issued. Vietnam need to learn the experiences from the other countries to developing specific legal regulations on chemical security to ensure Vietnam's legal regulations correspond and keep pace with international regulations. Herein discussion will be focused on the following points with the goal of developing the regulations on chemical security.

1. Experience in developing the legal regulations on Chemical supply chain security.
2. Experience in developing the legal regulations on the responsibilities of state management agencies and enterprises.
3. Experience in chemical security training and education.

Keywords: Chemical safety, chemical security, regulation

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SYSTEMATIC LITERATURE REVIEW: CHARACTERISTICS OF CONFINED SPACE HAZARDS IN THE CONSTRUCTION SECTOR

Kadir Arifin, Mohd Akhir Ahmad *, Azlan Abas, Mohamad Xazaquan Mansor Ali

Centre for Research in Development, Social and Environment (SEEDS), Faculty of Social Sciences and Humanities, The National University of Malaysia, 43650, Bangi, Selangor, Malaysia

Corresponding author: kadir@ukm.edu.my

Abstract

Background: Construction sector's employees are exposed to high risks when dealing with confined spaces at construction sites, as indicated by the high number of fatality cases. Confined spaces risk management is significantly impacted due to rapid technological advancements. To date, there are rudimentary studies with regards to confined spaces risk assessment in the construction sector. This paper proposes to conduct a comprehensive systematic literature review on the characteristics of confined space hazards in the construction sector. **Method:** The written text information is compiled from Scopus and Web of Science databases. The systematic literature review method was based on the preferred reporting items for systematic reviews and meta-analysis statements (PRISMA). This study attempts to highlight the hazard involved in the construction sector's confined spaces. **Results:** This study thoroughly reviewed 25 articles from the Web of Science and Scopus databases. **Conclusion:** The findings demonstrated that interested parties must develop short- and long-term adaptation strategies to manage confined space activities in the construction sector. The strategies include prevention techniques for confined space activities to proactively avoid severe injuries and fatalities, broadening the mitigation activities scope beyond atmospheric risks. Other recommendation includes providing information on specific areas and research content as part of future studies focus. This review also shows that atmospheric hazards as well as physical hazards involved in confined spaces need further attention to drive fatality cases reduction further in confined spaces.

Keywords: Atmospheric risk Occupational health and safety Enclosed environment Confined space Risk assessment Construction safety management

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CELEBRATING A CENTURY OF INNOVATION AND PARTNERSHIP: FROM TREES TO TECHNOLOGIES – 100 YEARS OF SHAPING THE GLOBAL RUBBER LANDSCAPE

Zairossani Mohd Nor¹, Kok Lang Mok², Fatimah Rubaizah Mohd Rasdi³

¹*Director General Office, 18th Floor Bangunan Getah Asli (Menara), Malaysian Rubber Board, 148 Jalan Ampang 50450 Kuala Lumpur, Malaysia.*

²*Deputy Director General Office, 18th Floor Bangunan Getah Asli (Menara), Malaysian Rubber Board, 148 Jalan Ampang 50450 Kuala Lumpur, Malaysia.*

³*Technology and Engineering Division Director Office, RRIM Sungai Buloh Research Station, Malaysian Rubber Board, 47000 Sungai Buloh, Selangor, Malaysia.*

**Corresponding author: zairossani@lgm.gov.my; klmok@lgm.gov.my; rubaizah@lgm.gov.my*

Abstract

This year, the Malaysian Rubber Board (MRB) proudly celebrates a century of pioneering leadership in rubber science, technology, and innovation. This legacy began with the establishment of the Rubber Research Institute of Malaysia (RRIM) in 1925, followed by the Tunku Abdul Razak Research Centre (TARRC) in 1938. In 1998, they were merged to form MRB, unifying the nation expertise in rubber research, development, and trade under a single agency. This keynote commemorates MRB century-long journey of transformative contributions that have shaped the global rubber industry across upstream, midstream, and downstream sectors. From early natural rubber tapping to advanced high-performance materials and sustainable practices, MRB has consistently driven progress through research, policy innovation, and international collaboration. The presentation will highlight MRB pivotal role in advancing Malaysia's economic development through breakthroughs in both natural and synthetic rubber, including innovations in technology, sustainability, and circular economy solutions. It will also explore how MRB integrates the Sustainable Development Goals (SDGs), into its R&D strategies. Looking ahead, this talk will outline MRB vision for the next century, with a focus on green technologies, the application of IR 4.0 in rubber research, smart materials, and safety. This centennial address honours MRB legacy while calling the global scientific community to co-create a more sustainable future for the rubber industry.

Keywords: Malaysian Rubber Board, Natural Rubber Technology, Synthetic Rubber Innovation, Rubber Industry Policy, Sustainable Rubber Ecosystems, IR 4.0 in Rubber Research.

PROPERTIES OF NANOCELLULOSE-ENHANCED CARBOXYLATED NITRILE BUTADIENE RUBBER (XNBR) LATEX FILMS

Nuur Syuhada Dzulkafly ¹, Norfatirah Muhamad Sarih ², and Azura A. Rashid ^{1,*}

¹ *School of Materials and Mineral Resources Engineering, Universiti Sains Malaysia,
Engineering Campus, 14300 Nibong Tebal, Seberang Perai Selatan,
Pulau Pinang, Malaysia.*

² *School of Chemical Sciences, Universiti Sains Malaysia, 11800 Gelogor, Penang, Malaysia.*

**Corresponding author: srazurea@usm.my*

Abstract

Carboxylated Nitrile Butadiene Rubber (XNBR) latex is increasingly used in glove manufacturing due to its superior strength and lack of proteins that trigger allergies. However, conventional crosslinking systems, such as sulfur and accelerators, may cause Type IV hypersensitivity and reduce the biodegradation rate of XNBR latex films. To address these challenges, nanocellulose has emerged as a promising alternative, functioning both as a biodegradable filler and a sustainable crosslinker. This study explores the incorporation of nanocellulose fibers (CNF) extracted from oil palm empty fruit bunches (OPEFB) into XNBR latex to improve biodegradation. The latex films were prepared with and without sulfur crosslinking, employing various formulations, including CNF, CNF-ZnO, CNF-ZDEC, and CNF-Sulphur. Conventional sulfur crosslinking served as a control. The prepared films underwent tensile testing, aging tests, and soil burial experiments to assess their mechanical properties and biodegradation rate. Results indicated that the absence of sulfur and accelerators in CNF-ZnO led to a minor reduction in tensile strength compared to the control film. Despite this, the tensile strength remained within acceptable limits for glove applications. Notably, the incorporation of CNF significantly enhanced the biodegradation rate, especially in the CNF-ZnO variant. Analytical techniques, including Fourier Transform Infrared (FTIR) spectroscopy, mass loss measurements, and surface morphology analysis, were utilized to monitor degradation over intervals of 2, 4, and 8 weeks during soil burial. The findings revealed that CNF-incorporated XNBR latex films exhibited significantly faster degradation compared to conventional XNBR films. Moreover, formulations without sulfur crosslinking degraded more rapidly than those with sulfur, emphasizing the impact of crosslinking chemistry on biodegradability. This study demonstrates the potential of using nanocellulose derived from agricultural waste as a sustainable solution to enhance the environmental performance of XNBR latex gloves.

Keywords: carboxylated nitrile butadiene rubber, nanocellulose fiber, biodegradation, crosslinking, agricultural waste

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ETHICS AND ACADEMIC INTEGRITY IN RESEARCH AND TEACHING

Uday Maitra

*Department of Organic Chemistry, Indian Institute of Science
Bangalore 560 012, India*

**Corresponding author: maitra@iisc.ac.in*

Abstract

The importance to follow ethical guidelines and maintaining academic integrity in Research and Teaching cannot be overemphasized.¹⁻³ During the past two decades it has become increasingly significant and relevant owing to the easy access to information through the internet. It is not unusual to hear about plagiarism, fabrication, and falsification of data in research publications/research proposals/students' reports etc. in many fields.⁴⁻⁶

This lecture will highlight the need to strictly follow ethical practices and maintain academic integrity in research and teaching at all levels. A few problem cases will also be discussed, along with some issues related to doing research.

Keywords: Ethics; academic integrity; research; education

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CHEMISTRY FOR GOOD: BRIDGING IUPAC PRINCIPLES AND LOCAL NEEDS IN ASEAN

Fun Man Fung

School of Chemistry, University College Dublin

**Corresponding author: funman.fung@ucd.ie*

Abstract

IUPAC is shaping a framework of guiding principles to promote responsible, sustainable, and inclusive chemistry. In the booming Southeast Asia region, where scientific research investment drives solutions to local challenges such as sustainability and industrial growth, these emerging principles offer a timely lens for regional advancement. This presentation explores their potential application in the Association of Southeast Asian Nations (ASEAN), founded in 1967 and currently has 10 member states. By using the future to build the present via a science diplomacy approach, it makes economic sense to connect ASEAN's local chemical innovation such as Singapore's specialty chemicals and Indonesia's agrochemical inputs with global goals. Drawing on partnerships like the OPCW's peaceful chemical security efforts and the United Nation's Sustainable Development Goals, I will highlight how chemists in the multicultural ASEAN states can adopt responsible chemical practices to support the greater good.

SUSTAINABLE AND INCLUSIVE CHEMISTRY LABS FOR A SUSTAINABLE FUTURE

Alejandra Palermo

Royal Society of Chemistry

Burlington House, Piccadilly, London, W1J 0BA, United Kingdom

**Corresponding author: palermoa@rsc.org*

Abstract

A truly sustainable future requires a holistic approach that integrates environmental responsibility, accessibility, and inclusivity. As a central science, chemistry plays a crucial role in addressing global sustainability challenges, including climate change, clean water, food security, and social equity. The United Nations Sustainable Development Goals (UN SDGs) call on the chemistry community to develop impactful solutions. Over the past 25 years, significant progress has been made, starting with the establishment of the 12 Principles of Green Chemistry in 1998. These principles laid the foundation for green chemistry as a distinct field, further solidified by key milestones such as the launch of the *Green Chemistry* journal in 1999. While chemists are actively working to reduce the environmental footprint of their research, laboratories remain resource- and energy-intensive spaces. Recognizing this, the Royal Society of Chemistry conducted a survey to assess sustainability efforts across academia and industry. However, sustainability goes beyond reducing waste and energy consumption—it must also ensure that scientific spaces are accessible to all. Sustainability isn't just about reducing carbon footprints—it's about ensuring that everyone has the opportunity to participate in scientific innovation. A truly sustainable future in the chemical sciences must address both environmental and accessibility challenges, ensuring that all scientists—regardless of background or ability—can contribute, innovate, and thrive. In this talk, I will explore chemistry's role in advancing sustainable laboratory practices and the urgent need for inclusive and accessible scientific spaces. By fostering a diverse and empowered workforce, we can drive innovation while ensuring that no one is left behind in shaping a sustainable future

Keywords: sustainable future, inclusion and diversity, disability inclusion

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BUILDING A RESPONSIBLE AND INCLUSIVE FUTURE IN CHEMISTRY

Javier Garcia-Martinez

Department of Inorganic Chemistry, University of Alicante, 03690, Alicante, Spain

**Corresponding author: j.garcia@ua.es*

Abstract

In recent years, the chemical sciences community has made remarkable progress in advancing professional and responsible practices, with a strong focus on fostering diversity, inclusion, and social responsibility. [1] In my presentation, I will highlight several key initiatives that are shaping a more equitable and sustainable future for chemistry. One such initiative is the IUPAC Global Women's Breakfast, an annual event that brings together women scientists from all career stages and disciplines across the world. By promoting networking, mentorship, and open dialogue, the Global Women's Breakfast strengthens communities of women in science and raises awareness of the barriers they face, while also celebrating their achievements. [2] I will also discuss the Gender Gap in Science Project, an ambitious undertaking coordinated under the International Science Council (ISC), which investigates gender inequalities across multiple scientific disciplines, including chemistry. [3] Through extensive data collection, surveys, and analysis, the project has provided critical insights into the challenges women and underrepresented groups face in STEM fields, helping to inform policies and initiatives aimed at narrowing the gap. In addition, I will present the IUPAC Guiding Principles for the Responsible Practice of Chemistry, a foundational document developed to promote ethics, integrity, and sustainability in chemical research and industry. A key aspect of these Guiding Principles is the emphasis on engaging diverse perspectives and promoting gender balance, recognizing that inclusive practices are essential for scientific innovation, societal relevance, and global impact. [4] By bringing together these efforts, the session will emphasize the importance of creating an environment where all individuals, regardless of gender or background, can contribute fully to the advancement of chemistry. These initiatives are not only vital for promoting fairness and equity but also for ensuring the resilience, creativity, and excellence of the scientific enterprise. [5] Ultimately, the presentation will underscore how embracing diversity, fostering inclusion, and adhering to responsible practices are critical to building a chemistry community that is better equipped to tackle global challenges and to drive scientific and technological progress for the benefit of all. [6,7]

Keywords: Ethics, IUPAC, gender balanced, Global Women Breakfast, diversity

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THE REACTION MEDIA AS “GREENING TOOL” IN THE SYNTHESIS OF PHOSPHORUS- AND SULFUR-CONTAINING POLYMERS

Natalia Tarasova^{a,*}, Alexey Zanin^a, Efrem Krivoborodov^a, Stanislav Karavaev^a,
 Nikita Ksenofontov^a, Timur Mirzaaliev^a, Pavel Shlyakhov^b, Pavel Sobolev^a,
 Diana Kirakosyan^a

^aDmitry Mendeleev University of Chemical Technology of Russia

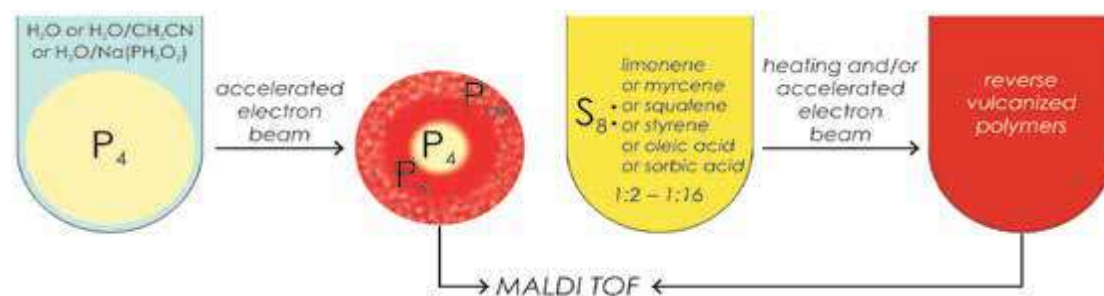
^bLomonosov Moscow State University

*Corresponding author: tarasova.n.p@mucrt.ru

Abstract

In recent years, novel functions have been developed for red phosphorus based materials, such as photocatalysis (benefiting from its narrow band gap of 1.5–2.4 eV) and secondary batteries (benefiting from its high theoretical specific capacity of 2596 mAh g⁻¹) [1]. However, despite the increasing range of applications, thermal methods for producing both red and white phosphorus are associated with the formation of by-products, as well as the risk of white phosphorus ignition upon contact with air [3]. To address these issues, this study examines the method of electron-beam-initiated polymerization of elemental phosphorus. However, a limitation of this method is the restricted penetration ability of electrons, which causes the reaction to occur only at the surface. To overcome this issue and reduce surface oxidation, the role of different reaction media was investigated. Recently, considerable attention has been paid to inverse vulcanization reactions. The inverse vulcanization process is based on the conversion of sulfur into a biradical form by heating it above 430 K, which requires certain energy costs. For this reason, a promising direction is the search for ways to modernize this technology, one of which is the use of high-energy radiation at the first stage of synthesis of sulfur-containing polymers with the selection of an organic crosslinking agent to set the operational properties of the final product. The dependence of conversion versus absorbed dose demonstrated that the addition of free radical acceptors increased the conversion rate by 7%, as the process of surface oxidation was delayed. A series of experimental studies was also conducted to identify the main patterns of the polymer formation process (thermal and/or electron beam initiated) with a high sulfur content, depending on environmental conditions and the use of various cross-linking agents, in particular: limonene, styrene, oleic acid, and sorbic acid.

Keywords: red phosphorus; ionizing radiation; accelerated electrons; polymers; reaction medium



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HARNESSING THE TINY PORES TO SOLVE THE BIGGEST CHALLENGES: SIMULTANEOUS CRITICAL METALS AND PURE WATER RECOVERY

Hamdy Maamoun Abdel-Ghafar^{a,*}

^a *Central Metallurgical Research and Development Institute (CMRDI), 1 Elflezat st, PO 87 Helwan, Cairo, Egypt.*

**Corresponding author: hamdy.maamoun@gmail.com*

Abstract

Freshwater scarcity and critical resource depletion are two of the most urgent global sustainability challenges. Utilizing membrane-based separation and purification technologies are a key player in solving such biggest global challenges that we are facing nowadays. A custom-oriented fabrication with a precise control of membrane fabrication process can generate multiple and simultaneous solution of water purification, critical elements recovery and gas separation. This work presents a dual-purpose membrane-based solution that addresses both: a novel photothermal membrane (P), membrane distillation (MD) or photothermal membrane distillation (PMD) system designed for simultaneous water purification and recovery of critical metals such as lithium. By precisely engineering membrane properties, we achieve selective separation that enables clean water generation through membrane distillation while concurrently extracting valuable metal ions. These membranes demonstrated unique features including self-repelling of salt accumulation, antimicrobial resistance, and robust performance against organic fouling during wastewater treatment. This approach paves the way for sustainable, decentralized solutions in resource-limited and environmentally stressed regions—delivering clean water and securing critical materials essential for green technologies. The research underscores the transformative potential of custom-fabricated membranes in tackling the water-energy-resource nexus.

Keywords: Critical metals, Photothermal membranes; Membrane distillation, water-energy nexus

BISMUTH-BASED PHOTOCATALYSTS FOR GREEN DEGRADATION OF PERSISTENT ORGANIC POLLUTANTS

Mirabbos Hojamberdiev*

Mads Clausen Institute, University of Southern Denmark, Alsion 2, 6400 Sønderborg, Denmark

**Corresponding author: mirabbos@mci.sdu.dk*

Abstract

Persistent organic pollutants (POPs) and pharmaceuticals and personal care products (PPCPs) are emerging water pollutants and pose significant environmental health risks due to their chemical stability, toxicity, and resistance to conventional water treatment processes. As an advanced oxidation process, heterogeneous photocatalysis is promising for detoxifying such water pollutants because of its mild operating conditions and efficiency. Bismuth-based compounds are an important class of visible-light-responsive photocatalysts and have received much attention owing to their appropriate band edge positions, band gaps for visible light absorption, high mobility of photogenerated charge carriers stemming from the well-dispersed Bi 6s orbital, layered structure, easily tailored morphology, and non-toxicity. In this study, we explored two types of bismuth-based compounds (bismuth tungstate and bismuth (oxy)iodides) for visible-light-driven degradation of organic pollutants. In the first part of this study, Zn^{2+} (0–22.5 at%) was partially substituted for Bi^{3+} in the Bi_2WO_6 lattice to enhance its photocatalytic activity. According to the Le Bail fits, the unit-cell volume is slightly reduced from 487.7 Å³ to 480.8 Å³ by the partial substitution of smaller Zn^{2+} (0.74 Å for CN = 6) for larger Bi^{3+} (1.03 Å for CN = 6) in the Bi_2WO_6 crystal lattice, and the solubility of Zn^{2+} in the Bi_2WO_6 lattice was found to be below 17.5 at%. Among the $\text{Bi}_{2-x}\text{Zn}_x\text{WO}_{6+\delta}$ photocatalysts, 2.5 at% Zn^{2+} -substituted Bi_2WO_6 exhibited a larger water oxidation photocurrent density (0.316 mA·cm⁻² at 1.23 V_{RHE}) and the highest photocatalytic activity for the photodegradation of PFH_xA ($k_1 = 0.012 \text{ min}^{-1}$). Liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF/MS) reveals that decarboxylation and defluorination are the main possible routes for the photodegradation of PFH_xA over $\text{Bi}_{2-x}\text{Zn}_x\text{WO}_{6+\delta}$ photocatalysts. In the second part, we explored the oxidative phase transition from bismuth iodide to bismuth oxyiodides by altering the temperature and time of thermal treatment. The effect of the bismuth iodide- to-bismuth oxyiodide phase transition on the efficiency of the photocatalytic removal of nitazoxanide was investigated in this study. Thermal treatment of BiI_3 at 375°C for 1 h yielded a $\text{BiOI}/\text{Bi}_4\text{O}_5\text{I}_2$ heterostructure, which showed an outstanding photocatalytic activity for nitazoxanide degradation with $k_1 = 0.051 \text{ min}^{-1}$ and $k_2 = 4.225 \text{ mg}\cdot\text{g}^{-1}\cdot\text{min}^{-1}$. The photodegradation of nitazoxanide over crystalline bismuth (oxy)iodide proceeds via hydrolysis into acetylsalicylic acid and the respective aminonitrothiazol, followed by the deacetylation and decarboxylation processes. These findings demonstrate the potential of tailored bismuth-based photocatalysts as green, efficient materials for the removal of structurally diverse and persistent water pollutants under visible-light irradiation.

Keywords: Photocatalysis, Bi_2WO_6 , BiOI, Persistent organic pollutants, Visible light absorption

CONVERSION OF BIOMASS, CO₂, AND WASTE PLASTICS INTO CHEMICALS AND FUELS

Buxing Han

Institute of Chemistry, Chinese Academy of Sciences, 100190, Beijing, China

**Corresponding author: hanbx@iccas.ac.cn*

Abstract

Biomass is abundant renewable carbon resource. Carbon dioxide (CO₂) is the main greenhouse gas, and it is also a renewable, abundant, and cheap C₁ feedstock. Synthetic plastics are indispensable materials in modern life. However, huge amount of waste plastics is produced each year. Use of CO₂, biomass, and waste plastics as carbon sources to produce fuels and value-added chemicals is of great importance for carbon neutrality and sustainable development of our society. In recent years, we are very interested in green chemistry, especially catalytic conversion CO₂, biomass, and waste plastics. In this presentation, I would like to discuss some of the recent results in our group on design of green catalytic systems and their application in conversion of CO₂, biomass, and waste plastics into valuable chemicals and fuels.

Keywords: Transformation, Carbon dioxide, Biomass, Waste plastics, Chemical, Fuel

BIOCATALYST FOR ECO-FRIENDLY AND SUSTAINABLE ZERO-WASTE LEATHER MANUFACTURING AND KERATIN WASTE VALORIZATION

Wycliffe C. Wanyonyi¹ and Francis J. Mulaa²

¹*Department of Mathematics, Actuarial and Physical Sciences, University of Kabianga,
P.O. Box 2030, 20200 Kericho, Kenya*

²*Department of Biochemistry, College of Health Sciences, University of Nairobi,
P.O. Box 30197 - 00100, Nairobi, Kenya.*

Abstract

Leather manufacturing involves conversion of raw skin and hides into leather (stable material) through series of mechanical and chemical operations. The leather industry has attracted public outcry due to severe environmental degradation, pollution and health risks. Currently the industry faces serious sustainability challenge due to extensive use of toxic chemicals and generation of huge hazardous waste. In order to overcome the hazards caused by toxic chemicals in tanneries, protect the environment, eliminate Green House Gases (GHG) emission and minimize the consumption of energy and water, we have isolated novel enzyme from unique micro-organisms that provides a realistic alternate for toxic sodium sulfide used in dehairing of hides/skins and responsible for over 80% of pollution load in tanneries. The novel enzyme allows for cleaner leather processing, reduces dehairing period by over 85%, eliminates pungent smell and yield high-quality leather that exhibit better qualities such as softness, strength, toughness and pliability. The application of novel enzyme in the dehairing effectively facilitates 100% recovery, recycling and valorization of all by-products (which includes, fats, fleshing keratin and proteins (WO 2016/159394A8)). In addition, keratin waste (including hair, feathers, fish scales, wool, skins cuttings etc) are further enzymatically hydrolyzed at ambient environmental conditions of temperature and pressure to yield high quality animal feeds rich in amino acids. Biocatalysis will usher in a Zero-waste tannery that allows for circular retrofitting by creating circular leather processing hubs in tanneries making them more profitable while protecting the environment. Application of enzyme technology in clean leather processing and Keratin Waste recycling strongly depends on allocation of financial resources and adequate in research, development and implementation of this potentially powerful technology. Piloting of this innovation at industrial level is highly recommended for commercialization of the technology.

NEW POLYMER FROM STARCH: HIGH VERSATILE GREEN MATERIALS

Francesco Trotta^a.

^aDepartment of Chemistry, University of Turin – Via Pietro Giuria 7, 10125 Torino -Italy.

**Corresponding author: francesco.trotta@unito.it*

Abstract

In the recent years, to face severe environmental and health concerns, limit greenhouse effects and improve the management of the foreseeable depletion of fossil resources, chemistry has moved towards the use of renewable resources for the production of energy and the synthesis of chemicals. It is also important to note that, unlike materials deriving from fossils, which are often concentrated in a limited part of the world, renewable raw materials could theoretically be produced and utilized everywhere, thus reducing or eliminating the dependence supplies of the Countries. These renewable raw materials come from various value chains, such as vegetable oils, fats, cellulose, starch, wood and biomass. Today many products are made from renewable raw materials, which often require less energy consumption and use safer and eco-friendly synthetic routes. These include textiles, cosmetics, medicines, building materials, dyes, lubricants, intermediates and (bio)-polymers [1].

Of particular interest is the production of polymer materials using renewable resources. In fact, polymers have a wide range of applications and are of crucial importance in modern society. In 2022 a global production of 400 million tons of different polymers was recorded. However, only about 1% is actually related to bio-polymers although a constant growth has been detected.

In this lecture I would like to share the results obtained over the last decades on the use of some starch derivatives i.e. cyclodextrins and linear dextrins to produce both cross-linked and branched polymers with an impressive number of applications including drug delivery systems, gene therapy, bioremediation, energy, membrane formation, cosmetics, smart fabrics, CO₂ capture, sustainable agriculture and many others. [2]. In addition, according to the fifth principle of green chemistry, toxic solvent-free production and even solvent-free synthesis are possible, thus making these new materials particularly appealing.

Keywords: Raw materials, renewable resources, starch derivatives, dextrins, cyclodextrins References

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REPROCESSING RESIDUES FROM ARTISANAL MINING IN THE AMAZON BASIN: FROM GREEN CHEMISTRY RESEARCH TO SUSTAINABLE BUSINESS MODELS

Juan Carlos F. Rodríguez-Reyes

Department of Chemical Engineering, Universidad de Ingeniería y Tecnología

**Corresponding author: jcrodriguez@utec.edu.pe*

Abstract

Our research, initiated by the generous PHOSAGRO/UNESCO/IUPAC Green Chemistry grant, delves into the intricate complexities of gold and silver leaching processes. Through this work, we gained a deeper understanding of the inherent inefficiencies within conventional cyanide leaching, paving the way for proposing novel ore pre-treatment strategies aimed at significantly reducing cyanide consumption and enhancing metal extraction yields. Leveraging this crucial knowledge, our focus shifted to a critically impacted region: the Amazon basin. Here, uncontrolled artisanal gold mining relentlessly contributes to deforestation and widespread mercury contamination, leaving behind vast environmental devastation. Our comprehensive study of current artisanal mining practices revealed that significant amounts of residual gold remain unrecovered within discarded tailings. Consequently, we designed and investigated a more sustainable alternative based on chloride leaching. This method proved remarkably more effective than cyanide leaching, particularly due to the presence of iron-containing minerals in the ore, which exhibit high reactivity towards chloride as a leaching agent. Laboratory-scale trials, conducted in both stirred tank and airlift reactors, consistently demonstrated high gold recovery efficiencies, ranging from 70% to 85%. Gold recovery was subsequently achieved through a robust cementation process utilizing zinc. This work has resulted in three patents and in the development of a viable business model, which proposes to allocate a portion of the revenue generated from reprocessing these valuable residues directly towards promoting vital reforestation activities within the Amazon basin. Overall, this work powerfully underscores the transformative role of seed funds in fostering impactful, green chemistry solutions for pressing environmental challenges.

Keywords: Mineral Processing, Extractive Metallurgy, Green Chemistry, Gold, Mining

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RENEWABLE AND BIODEGRADABLE MATERIALS FROM FURANIC PLATFORM CHEMICALS

Bogdan Ya. Karlinskii^{a*}

^a*Zelinsky Institute of Organic Chemistry*

^a*Tula State University*

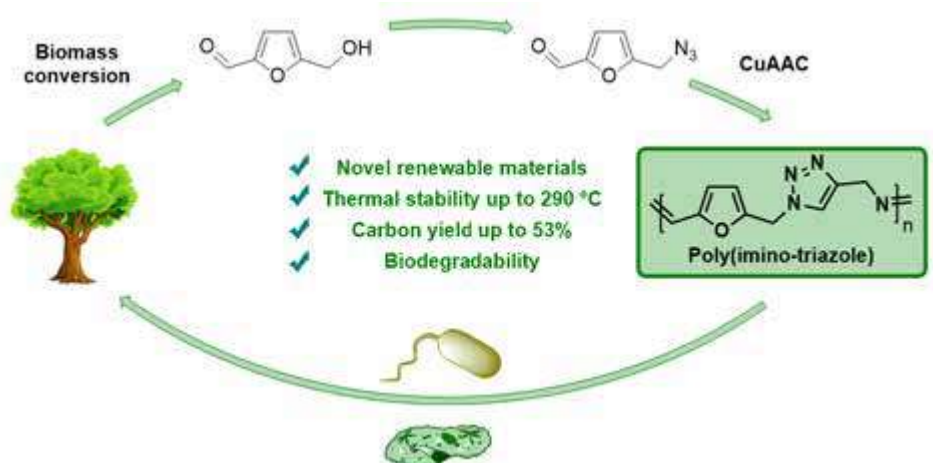
*Corresponding author: karbo@ioc.ac.ru

Abstract

Plant biomass is an almost limitless source of organic material that can be utilized as an alternative to fossil fuels to produce biofuels and base chemicals. Disubstituted furan-based platform chemicals, which are formed during the dehydration and aromatization of carbohydrates, are widely used as monomers for the production of various polymeric materials with diverse properties.^{1,2} In addition to their renewable nature, another interesting property of many of these materials is their ability to biodegrade under the influence of certain microorganisms.³ This is what distinguishes these polymers from their oil-based counterparts and is a significant advantage in the context of the growing problem of plastic waste accumulation around the world each year.

One of the more recent and interesting approaches to producing furan-containing polymers is through click polycondensation, which forms polytriazole chains.⁴ While this method currently has some limitations (such as low solubility of the materials and relatively low molecular weight), the potential for biodegradation of the resulting products is an incentive for continued research in this area.⁵

Keywords: biodegradability, platform chemicals, renewable polymers, 5-(hydroxymethyl)furfural



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SMART AND GREEN UTILIZATION OF BIORESOURCES – AN OPPORTUNITY FOR ACHIEVING A CIRCULAR ECONOMY

Vladimir Dimitrov

*Institute of Organic Chemistry with Centre of Phytochemistry,
Bulgarian Academy of Sciences*

**Corresponding author: vladimir.dimitrov@orgchm.bas.bg*

Abstract

The exploitation of available bioresources is a problem and a global task for humanity around the world to establish intelligent approaches to utilization. The resources we receive from nature should be treated according to the principles of green chemistry, expressed in the guiding motto “Conservation through Exploitation”. A significant portion of bioresources have been used for medicinal purposes for centuries. Even today, 80% of the world’s population uses plant-derived medicines for their healthcare. Currently, about 40% of the pharmaceutical products are based on natural compounds and traditional pharmacological knowledge. Natural resources are an inexhaustible source of bioactive compounds, preoptimized during the evolution, and therefore should be exploited with great attention and care.

The traditional use of natural raw materials and ethnopharmacological practices combined with the achievements of modern phytochemistry provide a wide range of opportunities for creating innovative products for everyday life. At the same time, the goal is to cultivate the necessary plants, deeply utilize the raw materials and process the waste to extract valuable biologically active substances. In this way, the principle of the circular economy could be realized. The current contribution will demonstrate some achievements in the application of traditional knowledge and modern chemistry for the use of bioresources in countries of Southeastern Europe.

Keywords: bioresources, circular economy

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CHARACTERIZATION AND VALORIZATION OF PLANT BIODIVERSITY AND NATURAL RESOURCES FOR MORE FOOD AND PHARMACEUTICAL SOVEREIGNTY AND SUSTAINABLE DEVELOPMENT IN AFRICA: THE KEY ROLE OF CHEMISTRY

Dogo SECK^a

^aNational Academy of Sciences and Technology of Senegal

^aCorresponding author: dogoseck@orange.sn / dogo.seck@ansts.sn

Abstract

Africa is rich in plant species and natural resources of great diversity, reflecting the continent's size and ecology. Unfortunately, these resources are insufficiently inventoried and characterized for their full exploitation in agriculture for food production and protection, health via phytomedicaments and industry by extracting essential oils and other metabolites from some species in order to ensure more sovereignty in these sectors and sustainable development. To this end, chemistry is a key discipline supporting collection of potential species, evaluation of their biological activity, identification and characterization of active ingredients, and the design of appropriate processes for the industrial exploitation of these endogenous resources.

Keywords: agriculture, bio pesticides, phytomedicaments, essential oil, Africa

SUSTAINABLE HEALTHCARE WITH BIO-BASED SMART POLYMERS

Lee Choy Sin^a

^a*Department of Pharmaceutical Chemistry, School of Pharmacy,*

^a*IMU University, Bukit Jalil, Kuala Lumpur.*

^a*Corresponding author: choysin_lee@imu.edu.my*

Abstract

The global polymers market is projected to reach USD 1,200 billion by 2032, with the medical polymers sector alone expected to grow at a 9.4% CAGR, reaching USD 31 billion by 2027. Simultaneously, the renewable chemicals market—including bio-based polymers—is anticipated to reach USD 316 billion by 2032, growing at an 11.2% CAGR. In parallel, the global smart polymer market is forecasted to grow significantly, reaching an estimated USD 80.53 billion by 2032. These intersecting trends underscore a timely opportunity to align material innovation with sustainability in the biomedical and pharmaceutical sectors. This talk will highlight the emergence of synthetic polymers derived from renewable feedstocks, developed using green chemistry principles. Bio-based polymers are not only biodegradable and biocompatible, but also highly tunable—enabling the design of smart, multi-responsive, and multi-functional systems for applications such as tissue engineering scaffolds, biomedical coatings, and pharmaceutical excipients. Experimental strategies employed to engineer these polymers, including the evaluation of their physicochemical, thermal, and mechanical properties will be discussed. The talk will also discuss current challenges in scaling up, regulatory hurdles, and balancing performance with sustainability.

VALORIZATION OF FOOD WASTE USING ALTERNATIVE STRATEGIES: CASE STUDY AT UFSM, BRAZIL

**Paola A. Mello^{a,*}, Alice P. Holkem^a, Thaís S. Berón^a,
Sandra K. Schlesner^b, Angélica I. Kaufmann^{a,b}, Juliano S. Barin^b**

^a Departamento de Química, ^b Departamento de Ciência e Tecnologia dos Alimentos, Universidade Federal de Santa Maria (UFSM), Santa Maria 97105-900, Brazil

*Corresponding author: paola.mello@ufsm.br

Abstract

In the global context of food being wasted or lost,^{1,2} researching strategies for valorisation is a matter of aligning the academy and society. Challenges and implications must be critically discussed to circumvent inherent drawbacks and reach the Sustainable Development Goals of the United Nations.³ Valorisation of plant-based residues, as from fruits and vegetables, accounts for a significant portion of food waste and appears to be a promising approach.^{4,5} Extraction of bioactive compounds using green extraction procedures (e.g., supercritical fluid extraction, pulsed electric fields, ultrasound-assisted extraction, microwave-assisted extraction, enzyme-assisted extraction, pressurized liquid extraction) are some green chemistry approaches that have been demonstrated mainly at laboratory scale for several kinds of residues. The research that is being developed at Federal University of Santa Maria, Brazil, is devoted to investigate the potential use of processes intensification alternatives, as ultrasound and microwaves, for food waste treatment and valorisation. The work plan included a survey of the loss during food production at the University Restaurant of UFSM, which produces about 7 thousand meals a day. Waste of beet, carrot, cabbage, chinese cabbage, tomato, and onion were separated to investigate valorisation processes. Samples were ground, frozen, and stored at -4 °C prior to experiments. The raw samples were characterised regarding moisture and ash content following standard protocols (AOAC 934.06 and AOAC 923.03, respectively) and general composition analysis was carried out following the respective AOAC protocols. Ultrasound apparatus that was investigated includes ultrasound bath operating at 20-80 kHz. Regarding the microwave technology, microwave hydro-diffusion and gravity (MHG) setup and cavity microwave oven were used. Processes conditions (as e.g. material: water ratio, temperature and time of treatment) were investigated. Composition (in terms of bioactive compounds) as well as the yield of extraction were critically compared and evaluated. The use of these wastes for prospecting products using 3-D printing of food is under development.

Keywords: food loss, process intensification, green extraction, ultrasound, microwave, 3-D printing.

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PITAYA-OIL BLEND POWDER WITH TWO IMPROVED FATTY ACID RATIOS: DEVELOPMENT AND CHARACTERIZATION

Zhi Xuan Yuo^{a*}, Swee Tee Thed^b

^a*Tunku Abdul rajman University of Management and Technology.*

^{*}*Corresponding author: yuozx-wl21@student.tarc.edu.my*

Abstract

Non-communicable diseases (NCDs) are responsible for 74% of all deaths worldwide, according to the World Health Organization (WHO) Report 2024. Dietary oils and fats with undesired fatty acid composition are linked to an increased risk of NCDs. The WHO recommended a SFA: MUFA: PUFA (saturated, monounsaturated, and polyunsaturated fatty acids) ratio at 1:1-2:1 for maintaining optimal LDL/HDL in the body. The omega-6: omega-3 (n-6: n-3) essential fatty acid ratio is important for health, with experts recommending a ratio of 1-4:1. This study aimed to develop pitaya-oil blend powder (POBP) with two improved fatty acid ratios using microencapsulation and spray-drying methods. The oil blend was first formulated using appropriate proportions of red palm oil, canola oil and algal oil. The oil blend achieved the desired SFA: MUFA: PUFA of 1:1.8:1 and n-6: n:3 of 1:1, both ratios supporting good health. The POBP exhibited relatively high antioxidant activity, with a $76.3 \pm 1.1\%$ ABTS radical scavenging capacity. Rancimat test at 120°C showed that the induction period of POBP (39.66 ± 0.21 h) was 18 times longer than that of the oil blend (2.19 ± 0.02 h), indicating that microencapsulation of oil blend with antioxidant pitaya extract significantly enhanced its oxidative stability. The overall color of POBP is pinkish orange ($L^* = 69.3$, $a^* = 19.5$, $b^* = 16.0$). The powder is slightly acidic (pH 5.29) with an Aw of 0.31, which favors microbial stability. The POBP demonstrated high solubility, indicating its potential application in foods and beverages. This project supports the Sustainable Development Goals SDG 3 – 3.4, targeting to reduce premature mortality from non-communicable diseases by one-third through prevention/treatment and promote health by 2030.

Keywords: red palm oil, algae oil, pitaya-oil blend powder, spray-drying, fatty acid ratios

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THE ROLE OF CATALYSIS IN THE IMPLEMENTATION OF GREEN CHEMISTRY AND SUSTAINABLE DEVELOPMENT: VIEW FROM MOSCOW

Lokteva Ekaterina S.^{a,*}

^a*Lomonosov Moscow State University, Russian Federation*

**Corresponding author: LES@kge.msu.ru*

Abstract

Catalysis has long been recognized as a cornerstone of green chemistry. This is mainly due to the high energy efficiency and selectivity of catalytic reactions, which reduce the environmental impact of chemical processes. In addition, these features make catalysis not only a safe, but also an economically viable choice. For these reasons, catalytic pathways are included as environmentally benign in the 12 principles of Green Chemistry. Catalysis is widely used in industrial processes, making them more atomically efficient and reducing their environmental impact. For example, petrochemistry, including polymerization processes, is largely based on catalytic technologies. However, there are still challenges in the implementation of catalytic processes in fine organic synthesis, pharmaceutical production and other industries. This presentation will review the successes and shortcomings in using catalysis to achieve sustainable development goals. In particular, the achievements of the Lomonosov Moscow State University staff will be presented.

Keywords: Catalysis, green chemistry, sustainable development, environment

As it is stated by IUPAC, ‘Catalyst is a substance that increases the rate of a reaction without modifying the overall standard Gibbs energy change in the reaction; the process is called *catalysis*.’¹ Catalysis is at the heart of one of the most important principles of green chemistry: ‘Catalytic reagents (as selective as possible) are superior to stoichiometric reagents’². The action of the catalyst is based on the fact that it opens a new reaction pathway in which the energy barrier of the limiting step is lower than in the non-catalytic pathway to the same product. In addition, among the three characteristics of the catalyst (activity, selectivity, stability), selectivity is the most important, which is provided by the special properties of the catalysts and leads to a reduction in the amount of process waste. Consequently, catalysis by default ensures the energy efficiency and atom economy of the process. It can be seen that the principle of catalysis is closely related to other principles of green chemistry. That is why catalysis was called as a cornerstone of a green chemistry.³

For these reasons, catalysis underlies many chemical processes. In the paradigm of sustainable development, we can mention two hypostases of catalysis: environmental catalysis, aimed at waste utilization and purification of air, water, and soil, and catalysis for “green” processes, providing more sustainable and environmentally friendly production (Fig. 1). Both branches of catalysis are actively used in industry, and a number of directions of such application are presented in Fig. 1.

The preparation of catalysts is often an environmentally unfavorable process whose life-cycle environmental impact can be significant. And not all catalysts can be classified as Green materials, especially if they include heavy and toxic metals. More promising variants of green catalysts are also listed in Fig. 1. Prospective directions of catalysis development are related to the introduction of catalytic processes in organic synthesis, biomass processing, energy production, including by means of unconventional effects - photocatalysis, electrocatalysis, microwave action, and others.

The report will present some examples of work in these areas, carried out by scientists of the Lomonosov Moscow State University.

In particular, work aimed at the catalytic treatment of wastewater from micro-ecotoxics (diclofenac as an example)⁴, new ways of catalytic production of chemical products based on the principles of green chemistry, and ways of catalytic processing of renewable raw materials will be described.

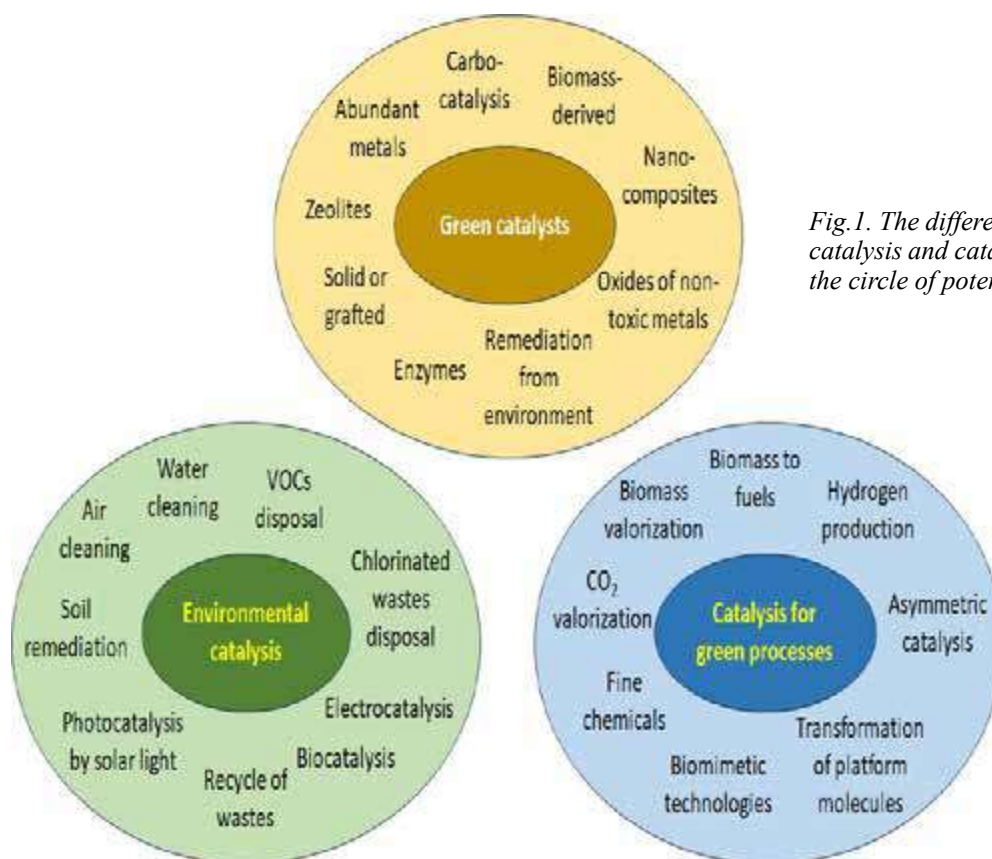


Fig. 1. The difference between environmental catalysis and catalysis for green chemistry, and the circle of potential green catalysts

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