สมาคมเคมีแห่งประเทศไทย
CHEMICAL SOCIETY OF THAILAND

FACS
FEDERATION OF ASIAN CHEMICAL SOCIETIES

20ACC
ASIACHEM2025
20th Asian Chemical Congress
June 23-27, 2025
Bangkok, THAILAND

Abstract E-book

www.acc2025thailand.com

Prof. Dr. Supa Hannongbua

Chairperson of the 20th Asian Chemical Congress
*(**20ACC**) or **ASIACHEM2025***

Message from the Chairperson of the 20th Asian Chemical Congress

On behalf of the organizing committee, I am delighted to welcome you all to the 20th Asian Chemical Congress (20ACC) or ASIACHEM2025, taking place from June 22nd to 26th, 2025, at the Berkeley Hotel Pratunam in the heart of Bangkok, Thailand.

For nearly four decades, the Asian Chemical Congress has served as a significant international platform in the field of chemistry, bringing together researchers and scientists from across Asia and around the world. It offers a valuable opportunity to present the latest research, exchange ideas, explore new scientific directions, and foster collaborations in both pure and applied chemistry.

The Chemical Society of Thailand jointly organizes the 20th Asian Chemical Congress (ACC) under the Patronage of Her Royal Highness Princess Chulabhorn Krom Phra Srisavangavadhana and under the auspices of the Federation of Asian Chemical Societies (FACS). We are also profoundly grateful for the generous support of various local and international organizations whose contributions have been instrumental in making this congress possible.

The 20ACC stands out for its emphasis on the theme "**Responsible Chemical Sciences for World Sustainability**," underscoring its greater significance in today's context. This congress is particularly well-aligned with the evolving role of chemistry and the chemical sciences in addressing pressing global challenges related to the environment, health, and energy.

The congress brings together almost nine hundred participants from both Thailand and abroad, representing 45 countries. Among the distinguished speakers are seven plenary lecturers, including Nobel Laureate in Chemistry (2004) Prof. Dr. Aaron Ciechanover, IUPAC President Prof. Dr. Ehud Keinan, and other renowned scientists. Additionally, approximately 200 invited speakers from 25 countries will share their expertise.

The latest advancements in chemical research, development, and education will be showcased across 11 regular sessions, 15 specialized symposia, and two side events designed to inspire and engage the younger generation with a passion for science. The program highlights progress in both pure and applied chemistry, emphasizing their contributions to technological innovation. Moreover, the congress will feature three poster presentation sessions and a comprehensive exhibition on chemicals and scientific instrumentation.

Organizing an event of this scale would not have been possible without the dedication and outstanding teamwork of many individuals who contributed generously in various capacities. I sincerely hope that the presentations and discussions held during the congress will foster continued academic advancement and promote deeper research collaboration both within the region and globally.

Notably, the congress also provided scholarships and valuable opportunities for young chemists and scientists to engage with leading experts in their respective fields, encouraging the exchange of knowledge and the passing of research experience from one generation to the next.

Aside from the congress, you will have the chance to experience a myriad of Thailand's exceptional and exotic tourist and cultural attractions. You will find the congress both valuable and enjoyable.

Last but not least, I am confident that, with your active participation and valuable contributions, the 20th Asian Chemical Congress will be among the most successful in its history. I sincerely wish you a memorable and rewarding experience during your stay in Bangkok.

With warmest regards,

Prof. Dr. Supa Hannongbua
Chairperson of the 20th Asian Chemical Congress (20ACC) or
ASIACHEM2025

Prof. Dr. Vudhichai Parasuk

President of Chemical Society of Thailand

Message from the President of the Chemical Society of Thailand

It is my great pleasure to welcome you to the 20th Asian Chemical Congress (20ACC) and to host the 22nd FACS General Assembly, which takes place from June 22 to 26, 2025, at The Berkeley Hotel Pratunam in the vibrant city of Bangkok, Thailand. This prestigious biennial event brings together chemists and researchers from across Asia and around the world to share their latest discoveries and innovations.

As President of the Chemical Society of Thailand, the proud host of this year's congress, I am honored to welcome you to what promises to be an inspiring and intellectually enriching event. The 20ACC serves as a premier platform for presenting groundbreaking research, fostering international collaborations, and cultivating lasting professional networks across all areas of chemistry.

In addition to the academic exchange, Bangkok offers a remarkable experience with its rich cultural heritage, renowned hospitality, and an array of leisure and culinary delights. We encourage you to take some time to explore and enjoy all that this dynamic city has to offer.

I wish you productive discussions, meaningful connections, and a memorable experience both at the congress and throughout your stay in Thailand.

With warmest regards,

Professor Dr. Vudhichai Parasuk
President of the Chemical Society of Thailand

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AC: Analytical Chemistry

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CE: Chemistry for Energy and Environment

Chair: Metta Chareonpanich	Kasetsart University, Thailand
Co-chair: Waleeporn Donphai	Kasetsart University, Thailand

FA: Food, Agriculture, and Cosmetics

Chair: Sirirat Kokpol	Chulalongkorn University, Thailand

FE: Future in Chemical Education

Chair: Taweetham Limpanuparb	Mahidol University, Thailand
Co-chair: Usa Jeenjenkit	Amnuay Silpa School, Thailand
Co-chair: Narisra Komalawardhana	Institute of Molecular Biosciences, Mahidol University, Thailand

IC: Inorganic Chemistry

Chair: Ekasith Somsook	Mahidol University, Thailand

IE: Industrial and Engineering Chemistry

Chair: Tawan Sooknoi	King Mongkut's Institute of Technology Ladkrabang, Thailand

MN: Materials Science and Nanotechnology

Chair: Vinich Promarak	Vidyasirimedhi Institute of Science and Technology, Thailand

NB: Natural Products, Biological Chemistry and Chemical Biology

Chair: Vatcharin Rukachaisirikul	Prince of Songkla University, Thailand

OM: Organic Synthesis and Medicinal Chemistry

Chair: Tirayut Vilaivan	Chulalongkorn University, Thailand

PC: Polymers and Bio-based Materials

Chair: Suwabun Chirachanchai	Chulalongkorn University, Thailand

PT: Physical and Theoretical Chemistry

Chair: Nawee Kungwan	Chiang Mai University, Thailand
Co-chair: Supareak Praserthdam	Chulalongkorn University, Thailand

SCIENTIFIC SESSIONS: SPECIAL

S1: Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy

Chair: Seiji Mori	Ibaraki University, Japan
Co-chair: Siriporn Jungsuttiwong	Ubon Ratchathani University, Thailand
Co-chair: Yoichi M. A. Yamada	RIKEN, Japan
Co-chair: Pinit Kidkhunthod	Synchrotron Light Research Institute, Thailand

S2: Catalytic Systems for Contemporary Challenges

Chair: Chularat Wattanakit	Vidyasirimedhi Institute of Science and Technology, Thailand
Co-chair: Thidarat Imyen	Kasetsart University, Thailand
Co-chair: Supawadee Namuangruk	National Science and Technology Development Agency, Thailand

S3: Advanced Coordination Materials and Catalysis for Environment

Chair: Jan J. Weigand	Technische Universität Dresden, Germany
Chair: Yasuhiro Funahashi	Osaka University, Japan
Co-chair: Nobuto Yoshinari	Osaka University, Japan
Co-chair: Dong-Myeong Shin	University of Hong Kong, Hong Kong

S4: Understanding and Development to Address the PFAS Problems in Thailand for Sustainable Environment (in Thai)

Chair: Chongrak Polprasert	Thammasart University, Thailand
Co-chair: Suratsawadee Sukeesan	Kasertsart University, Thailand
Co-chair: Amornpon Changsuphan	Department of Science Service, Thailand

S5: AI in Drug Discovery Research

Chair: Pornpan Pungpo	Ubon Ratchathani University, Thailand
Co-chair: Patchreenart Saparpakorn	Kasetsart University, Thailand

S6: Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia

Chair: Yodchai Tangjaideborisut	Chief Executive Officer at Food Matrix Global Co., Ltd., Thailand
Co-chair: Kampol Poophawatanakij	Medical director at Food Matrix Global Co., Ltd., Thailand

SCIENTIFIC SESSIONS: SPECIAL (cont.)

S8: Green Chemistry; Paving the Way to a Sustainable Future

Chair: Supakorn Boonyuen	Thammasat University, Thailand

S9: Ryoji Noyori ACES Symposium

Chair: Dinesh Talwar	Asian Chemical Editorial Society (ACES)

SA: Young Career Development under FACS-ACS Collaboration

Chair: Monthip Sriratana Tabucanon	Chemical Society of Thailand, Thailand
Co-chair: Ittipat Meewan	Mahidol University, Thailand

SB: TU-Frontier Lab-JEOL joint session Contaminants of Emerging Concern: PFAS & Microplastics

Chair: Chanatip Samart	Thammasat University, Thailand
Co-chair: Karthikeyan Sathrugnan	Frontier Laboratories, Singapore

SC: Sustainable Chemistry Focusing on Clean energy Good Health and Well-Being (Thailand-Taiwan)

Chair: Suwadee Kongparakul	Thammasat University, Thailand
Co-chair: Shuchen Hsieh	National Sun Yat-sen University, Taiwan

SD: IMS-CU Bilateral Symposium for Driving Forward Frontier Research

Chair: Kanet Wongravee	Chulalongkorn University, Thailand
Co-chair: Boodsarin Sawatlon	Chulalongkorn University, Thailand

SE: Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology

Chair: Priyani Paranagama	University of Kelaniya, Sri Lanka
Co-chair: Suranga Wickramarachchi	University of Kelaniya, Sri Lanka

SG: Sustainable Chemistry for Agricultural Residue Valorization

Chair: Kuntawit Witthayolankowit	Kasetsart University, Thailand
Co-chair: Sunisa Akkarasamiyo	Kasetsart University, Thailand

SCIENTIFIC SESSIONS: SIDE-EVENTS

SS: Science Projects for Students Showcase

Chair: Peera Atcharasathian	Thammasat University, Thailand
Co-chair: Supakorn Boonyuen	Thammasat University, Thailand

US: Future Chemistry Research Presentation for High School Students

Chair: Siwaporn Meejoo Smith	Mahidol University & ACS Thailand Chapter, Thailand
Co-chair: Supakorn Boonyuen	Thammasat University, Thailand

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PLENARY ABSTRACTS

Plenary Session (PL-1)

Humanity faces a bright future, and so Chemistry

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Humanity faces six global challenges: 1) Climate change and air quality, 2) Sustainable energy, 3) Dwindling raw materials, 4)Water scarcity and safety, 5) Food for everybody, 6) Health problems.

These problems are complex because they cannot be solved by known technologies, but future technologies will solve them. Because all six problems are primarily chemical issues, it is our responsibility and opportunity, as chemists, to meet these challenges. Everything is chemistry, and all sciences are chemistry because they all deal with matter, and all matter is made of atoms and molecules.

Humanity faces a bright future due to four reasons: 1) Knowledge explosion, 2) Unpredictability of science, 3) Evolution of network society, 4) Human spirit and creativity. We live in artificial environments, eat genetically engineered food, wear synthetic and genetically modified fibers, and travel by fabricated devices. In other words, we live on products of human imagination and creativity, and since imagination and creativity have no limits, the effective area of planet Earth has no limits.

Therefore, the best ways to meet global challenges are: 1) Invest in education at all levels – encourage curiosity, 2) Invest in basic, high-risk, exploratory science, 3) Bolster human liberty, dignity, and democracy, 4)Encourage economic growth because only rich countries can afford good education, health, scientific innovation, and adaptation.

Keywords: global challenges; chemistry; future technologies; human creativity; education and innovation

President of the Israel Chemical Society (second term), Editor-in-Chief of the Israel Journal of Chemistry (published by Wiley-VCH), and President of the International Forum of Bio-Inspired Engineering (IFBIE, Boston, USA). He was the founder of two startup companies based on his technologies. He was the founder and first Head of the Institute of Catalysis Science and Technology (ICST) in the Technion. Member of the Executive Board of EuCheMS and Chairman of the Advisory Council of High School Chemistry Education, Ministry of Education.

Plenary Session (PL-2)

Construction and application of self-assembled nanostructures

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Self-assembled nanostructures represent a critical frontier in nanoscience, integrating principles from physical, inorganic, polymer, and materials chemistry. In our research, we have uncovered fundamental mechanisms governing the self-limited assembly of polydisperse building blocks into uniform nanostructures. By leveraging these insights, we have developed precise methods for constructing functional nanoporous composites and demonstrated their high performance in catalytic and membrane separation applications.

Keywords: self-assembled nanostructures; polydisperse building blocks; nanoporous composites; catalytic applications; membrane separation

Zhiyong Tang is a professor at the National Center for Nanoscience and Technology, China, specializing in self-assembled functional nanomaterials for energy and environmental applications. He earned his Ph.D. from the Chinese Academy of Sciences and completed postdoctoral research in Switzerland and the U.S. Tang has published over 400 high-impact papers with more than 46,000 citations. His honors include the National Natural Science Award (2018), TWAS Chemistry Award (2019), and election to the Chinese Academy of Sciences (2023).

Plenary Session (PL-3)

Ubiquitin proteolytic system - From basic mechanisms thru human diseases and on to drug development

Aaron Ciechanover*

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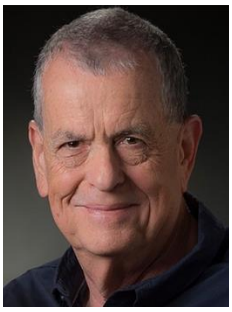
Between the 50s and 80s, most studies in biomedicine focused on the central dogma - the translation of the information coded by DNA to RNA and proteins. Protein degradation was a neglected area, considered to be a non-specific, dead-end process. While it was known that proteins do turn over, the high specificity of the process - where distinct proteins are degraded only at certain time points, or when they are not needed any more, or following denaturation/misfolding when their normal and active counterparts are spared - was not appreciated. The discovery of the lysosome by Christian de Duve did not significantly change this view, as it was clear that this organelle is involved mostly in the degradation of extracellular proteins, and their proteases cannot be substrate-specific. The discovery of the complex cascade of the ubiquitin solved the enigma. It is clear now that degradation of cellular proteins is a highly complex, temporally controlled, and tightly regulated process that plays major roles in a variety of basic cellular processes such as cell cycle and differentiation, communication of the cell with the extracellular environment and maintenance of the cellular quality control. With the multitude of substrates targeted and the myriad processes involved, it is not surprising that aberrations in the pathway have been implicated in the pathogenesis of many diseases, certain malignancies and neurodegeneration among them, and that the system has become a major platform for drug targeting.

Keywords: ubiquitin; protein degradation; cellular quality control; lysosome; drug targeting



Aaron Ciechanover is a Distinguished Research Professor at the Technion – Israel Institute of Technology. He earned his M.Sc. (1971) and M.D. (1973) from the Hebrew University in Jerusalem, and completed a D.Sc. at the Technion in 1982. His work revealed that ubiquitin-mediated proteolysis is vital for numerous cellular processes and is implicated in various diseases. Among the numerous prizes Ciechanover received are the 2000 Albert Lasker Award, the 2002 EMET Prize, the 2003 Israel Prize, and the 2004 Nobel Prize (Chemistry; shared with Drs. Hershko and Rose). He is a member of the Israeli National Academy of Sciences and Humanities, the American Academy of Arts and Sciences (Foreign Fellow), among others.

Plenary Session (PL-4)

Translational chemical biology

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Many critical biological processes are conducted by small molecules, so they can arguably be regarded as another essential component of the "central dogma" of molecular biology. Biologically meaningful small molecules may be natural products discovered by nature through many cycles of diversity generation and natural selection, or they may be prepared through organic synthesis to develop drug candidates or chemical probes to study life's processes. Accordingly, the central theme of our research focuses on the efficient synthesis of these small molecules and the subsequent biological evaluations of these molecules by applying medicinal chemistry and chemical biology approaches. This lecture will illustrate the opportunities at this interface between chemical biology and drug discovery by describing a series of examples we are actively working on in our laboratory at Peking University. We extensively use bioactive small molecules to explore new biology and develop novel drug candidates for human diseases, such as cancers and autoimmune diseases.

Keywords: chemical biology; natural product; chemical genetics; drug discovery

Prof. Xiaoguang Lei is the Boya Distinguished Professor of Chemistry and Chemical Biology at Peking University and a senior PI at the Peking-Tsinghua Center for Life Sciences. His research focuses on chemical biology, natural product synthesis, synthetic biology, and drug discovery. He has published over 180 papers in top journals like Science, Cell, and Nature, and holds 20 patents. Prof. Lei has developed four first-in-class drug candidates, with one in Phase II clinical trials. He has received numerous prestigious awards, including the 2023 Sackler Chair Visiting Scholar Award and the 2022 MDPI Tu Youyou Award.

Plenary Session (PL-5)

Sustainability and homogeneous catalysis of organic reactions: Aspects of nickel, copper, silver and gold

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Following some early observations, Ostwald and later Berzelius defined the concept of Catalysis. Today, catalysis is a key technology of chemical production, improving selectivity and lowering the barrier of activation for reactions. At least 80% of all processes involve catalysis. Thus, future sustainability improvements will also rely on the progress of catalysis research.

The presentation will discuss and exemplify different factors for this future task. For selected recent examples of nickel, copper, silver and gold catalysis this will be analyzed. Catalyst preparation, methodology development, and mechanistic studies including computational chemistry are important elements of this discussion.

Applications of these reactions cover materials science as well as aspects of pharmaceutical chemistry.

Keywords: catalysis; nickel; copper; silver; gold

Born 1963, Ph.D. from LMU Munich (1991) with G. Szeimies. Postdoc with B.M. Trost at Stanford (1991-1993). Assistant Professor with J. Mulzer at Free University of Berlin, University of Frankfurt and University of Vienna. Visiting Scientist at the University of Tasmania (1999). Temporary Professorship at Marburg University (1999), Associate Professor at Stuttgart University (Associate Professor, 2001), Full Professor at Heidelberg University since 2007. Dr. Otto Röhm Memorial Fellowship (1998); Karl-Ziegler Memorial Fellowship (2001), ORCHEM Prize for natural sciences of the German Chemical Society (2002); Hector Research Prize 2010.

Plenary Session (PL-6)

Enzyme catalysis for green synthesis

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Enzymes or biocatalysts are important for development of green processes such as synthesis of pharmaceuticals and applications in food and environmental technologies. However, biocatalysts are often less stable or not functional under the conditions required by industries; they thus require proper engineering to fine-tune activities for serving industrial requirements. Here, we will discuss our recent work in mechanistic studies, enzyme engineering, biocatalysis and applications of halogenase, oxidase, monooxygenase and decarboxylase. Our recent mechanistic studies of a single-component flavin-dependent halogenase has elucidated the important roles of ligands in regulating the catalytic cycle of the halogenase, especially the use of $NADP^+$ as a turn-on switch for halogenation and the use of organic substrates to accelerate a reset process to prepare the enzyme for next catalytic cycles. We have used a strategic design and combined use of *in silico* tools to improve thermostability of tryptophan monooxygenase. The reaction of tryptophan monooxygenase is important for plant hormone synthesis. We used semi-rational enzyme engineering and machine learning approach to engineer a phenolic hydroxylase to be enantio-selective and demonstrated the use of engineered enzyme for synthesis of catecholic drugs. On the last topic, we used ancestral sequence reconstruction to create decarboxylases which can be used in chemo-enzymatic C-C bond coupling reactions.

Keywords: enzyme; biocatalysis; chemo-enzymatic reaction; enzyme engineering; halogenase

Pimchai Chaiyen is President of Vidyasirimedhi Institute of Science and Technology (VISTEC), and a professor at School of Biomolecular Science and Engineering. Her research spans enzyme catalysis, enzyme engineering, systems biocatalysis, metabolic engineering, and synthetic biology, focusing on elucidating enzymatic mechanisms, discovering novel enzyme functions, and reprogramming metabolic pathways. She has received numerous honors, including the L'Oréal-UNESCO Woman in Science Crystal Award (2017) and Thailand's Outstanding Scientist Award (2015), and currently serves as Associate Editor for ACS Catalysis.

Plenary Session (PL-7)

Nanoengineered materials and coatings for medicine and beyond

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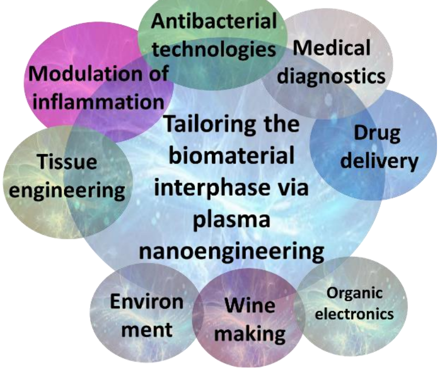
In this plenary talk, I will give an overview of recent progress from my lab on development of plasma polymer facilitated nanoengineered surfaces and materials that benefit many areas of application. Over the years, we developed a range plasma-based methods with allows us to control that entire spectrum of material surface properties, including chemical, physical, mechanical and topographical. The main focus of our research is the design and surface modification of novel medical devices and biomaterials for applications in areas such as tissue engineering, controlling inflammation and infections, drug delivery and medical diagnostics. However, our surface modification technologies are not limited to medicine. We have demonstrated the utility of nanoengineered plasma polymers for solving problems in other areas such as environmental science and remediation, water treatment and even wine making. I will present the engineering and chemical concepts underpinning "plasma nanoengineering" and give a range of examples of application of the technology in various fields, including commercial applications.

Keywords: plasma; medical devices; antibacterial surface; infection; tissue engineering

Applications of Plasma Nanoengineering



Krasimir Vasilev earned his Ph.D. from the Max Planck Institute for Polymer Research in 2005. He is now a Matthew Flinders Professor, NHMRC Leadership Fellow, and Director of the Biomedical Nanoengineering Laboratory at Flinders University. His research focuses on biomedical nanoengineering, securing over $25M in funding and publishing 330+ papers with 14,000+ citations (h-index 65). He has received multiple prestigious fellowships and awards, including from the ARC, NHMRC, Humboldt Foundation, and the John A. Brodie Medal for achievements in Chemical Engineering.

Plenary Session (PL-8)

Empowering teachers, inspiring youth: Driving sustainability through innovative small-scale chemistry in South Asia and ASEAN

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Access to practical science education remains a significant barrier for students in many parts of the world, particularly in South Asia and Southeast Asia, where traditional laboratory instruction is often hindered by safety concerns, high costs, and limited infrastructure. This plenary talk presents a decade-long initiative that introduces Small-Scale Chemistry (also known as microscale chemistry) as an innovative, safe, and sustainable teaching approach for secondary schools across the region. The method enables meaningful hands-on learning through the use of minimal chemicals and portable tools, while also empowering teachers to become catalysts for educational transformation within their communities. Case studies and regional outcomes will demonstrate how this approach reduces educational inequities, promotes environmental awareness, and aligns with key UN Sustainable Development Goals. The session will explore practical impacts, cross-border collaboration, and future directions for broader integration—ultimately advocating for inclusive, inspiring science education as a driver of long-term sustainability.

Keywords: teacher empowerment; small-scale chemistry; educational equity; sustainable development goals; South Asia and Southeast Asia

Supawan Tantayanon is a professor at Chulalongkorn University, recognized for her contributions to green chemistry, chemical safety, and science education. She has held key positions in many organizations, including President of the Science Society of Thailand, the Council of Science and Technology Professionals of Thailand, the Chemical Society of Thailand, the Polymer Society of Thailand, the Federation of Asian Chemical Societies, and the Pacific Polymer Federation. Internationally recognized for pioneering Small-Scale Chemistry and developing "Small Lab Kits," she promotes safe, low-cost, and eco-friendly science education. Her many honors include the IUPAC Distinguished Women in Chemistry Award (2021). She continues to advise UNESCO and the OPCW, advancing inclusive and sustainable science education in South Asia, Southeast Asia, and beyond.

KEYNOTE ABSTRACTS

Physical and Theoretical Chemistry (PT-K-004)

GenAI for autonomous chemistry labs

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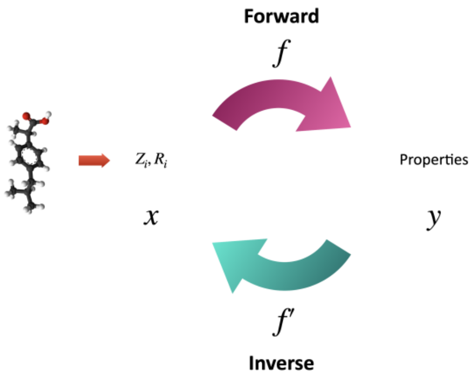
In recent years, modern AI/ML methods have revolutionized and have had phenomenal success in many technology areas such as computer vision, natural language processing, machine translation, speech recognition, autonomous driving, etc. Availability of high performance GPU accelerators, historical data and development of new algorithms/libraries have fueled such a surge. This has inspired chemists and biologists to apply these algorithms to problems in molecular science that are traditionally tackled using physics-based methods. The past few years have witnessed ML based solutions in molecular science that are more efficient and accurate compared to traditional methods. In this talk, I will initially introduce the philosophy of machine learning methods in the context of the three paradigms of research (experiments, theory and computations). I will also introduce the direct and inverse problems in the context of molecular/material design. In the second part of the talk, we will discuss inverse problem solving and explore some methods that may enable self-driving (autonomous) chemistry laboratories. We will discuss methods that are capable of generating novel molecules based on a chemist's requirement (like ChatGPT for text), and how AI is capable of elucidating structures given molecular spectra as inputs. Finally, we will briefly discuss how the informatics based approaches could impact the way we do research in computational molecular science.

Keywords: artificial intelligence; machine learning; generative AI; self-driving labs



Deva (b. 1977) is a Professor and Head of the Center for Computational Natural Sciences and Bioinformatics at IIIT Hyderabad, and Project Director of IHub-Data. He earned his Ph.D. from Pondicherry University/IICT Hyderabad and completed postdoctoral research at the University of Maryland. His work focuses on applying computational methods to chemical and biological systems. He has received numerous honors, including the INSA Young Scientist Medal, CRSI Medal, JSPS Fellowship, and Google Impact Scholar Award.

Physical and Theoretical Chemistry (PT-K-012)

A novel enzymatic reaction mechanism analysis method using QM/MM MD

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Currently, QM/MM MD simulations have become an important tool for elucidating enzyme-catalyzed reaction mechanisms, predicting catalytic sites, and guiding catalyst design. [*Biochemistry* **2013**, *52*, 2708–2728] However, due to the high computational cost, the timescales accessible by QM/MM MD simulations are much shorter than those of actual enzyme-catalyzed reactions. This makes it impractical to directly observe the entire reaction process, especially the breaking and forming of chemical bonds, using QM/MM MD simulations. To address this issue, various enhanced sampling methods have emerged. However, traditional sampling methods have a critical drawback: they require users to pre-define collective variables that describe the entire reaction process. In enzyme-catalyzed reactions, a nucleophilic attack or SN2 reaction is often accompanied by multiple proton transfers. Even experienced researchers may find it challenging to determine the sequence of these steps and to ascertain whether the reaction proceeds stepwise or in a concerted manner, making it difficult to accurately predict key structures along the reaction pathway and the corresponding energy barriers.

To overcome these limitations, we have developed and applied the PaCS-Q method, [*Journal of Chemical Theory and Computation* (submitted)] which accelerates the exploration of reaction pathways without relying on external restraints or pre-defined reaction coordinates (Fig. 1). PaCS-Q performs time-resolved sampling of the breaking and forming of chemical bonds, effectively identifying transition states and intermediates in complex biochemical reactions. To validate the performance of PaCS-Q, we applied it to two case studies: (i) the Claisen rearrangement reaction catalyzed by chorismate mutase and (ii) the peptide aldehyde reaction in the NS2B/NS3 serine protease of the Zika virus. The results demonstrate that PaCS-Q not only captures critical mechanistic details of both stepwise and concerted processes but also significantly reduces computational costs compared to traditional enhanced sampling techniques.

Keywords: QM/MM; parallel cascade selection MD; free energy; enzymatic reaction analysis

Prof. Yasuteru Shigeta is a Theoretical Chemist working at University of Tsukuba as a full professor since 2014. He has published more than 350 scientific papers and received the PCCP award of Royal Society of Chemistry (UK) in 2007, Young-chemists award of the Chemical Society of Japan in 2009, the Young-scientists award of Ministry of Education, Culture, Sports, Science, and Technology (MEXT) Japan in 2010, the Young-scientists award of Japan Society for Molecular Science in 2012, and the QSCP Promising Scientist Prize of CMOA in 2017.

Chiral molecules and solids for spintronics

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Chirality-Induced Spin Selectivity (CISS) is attracting recent attention as a new source of spin polarized current. It also provides unique methods for enantio-separation, [*Science* **2018**, *360*, 1331] enantio-selective electrochemical reactions, and efficient water oxidation. The mechanism of CISS effect is, however, yet to be clarified, as the effect is much larger than expected one estimated with small spin-orbit coupling for organic molecules. In a hypothetical consideration, it is proposed that an enhancement of spin polarization is associated with anti-parallel spin pair at two opposite ends of a chiral molecule. [*Science* **2018**, *360*, 1331] It is interesting to note that such an anti-parallel spin pair is a time-reversal (T) odd state, while the chiral molecular structure is T-even. We think symmetry conversion from T-even to T-odd quantities gives an essential clue to understand CISS effect that can generate huge spin polarization in a non-equilibrium condition.

We have made such a symmetrical consideration based on multipole basis and found that a T-odd chirality can emerge from an accumulation of spin current at reservoirs. [*Isr. J. Chem.* **2022**, *62*, e202200049] In a chiral metal, we have confirmed that the CISS effect appears as spin polarization [*Appl. Phys. Lett.* **2020**, *117*, 052408] rather than spin filtering. In addition, we have shown that chiral organic superconductors can exhibit spin accumulation at two opposite crystal edges whose directions are anti-parallel to one another. [*Nature* **2023**, *613*, 479] This can be regarded as a macroscopic-size emulation of chiral molecules that has T-odd spin pairs at their opposite ends. A connection to falsely chiral influence [*Chem. Soc. Rev.* **1986**, *15*, 189] will be also discussed.

Keywords: chiral materials; superconductor; spintronics; CISS effect

Hiroshi Yamamoto received his D.Sc. in solid state chemistry at the University of Tokyo in 1998. He spent one year as an assistant professor at the Department of Physics, Gakushuin University, and 13 years as a research scientist at RIKEN. Since 2012, he has served as a full professor at the Institute for Molecular Science, National Institutes of Natural Sciences in Japan. His research interests focus on organic electronics and spintronics based on novel operation mechanisms. Organic superconductor transistors and spintronic devices based on chirality are two major current topics in his study.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-K-002)

Low-temperature sintering of sub-oxidized copper nanoparticles for power device

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The increasing demand for high-performance, low-cost conductive and sintered bonding materials has driven interest in copper as an alternative to silver. While copper offers excellent conductivity and affordability, its tendency to oxidize presents challenges for low-temperature sintering. This study explores the use of slightly oxidized copper nanoparticles ($Cu_{64}O$ and Cu_8O) to enhance sinterability.

Copper suboxide nanoparticles were synthesized using a chemical reduction method with hydrazine, with particle sizes controlled from a few nanometers to 200 nm. These nanoparticles transition to metallic copper below 100°C, facilitating atomic diffusion and enabling low-temperature sintering. Core-shell structures, where copper nanoparticles are coated with suboxide shells, were synthesized and analyzed using TEM and XRD. These structures promote strong bonding, achieving shear strengths up to 100 MPa after sintering at 200°C.

High-concentration conductive pastes were formulated, demonstrating excellent conductivity (10.7 μΩ•cm) and potential for large-scale production. Further research aims to optimize dispersion media, suppress cracking, and refine process control. This study establishes copper suboxide nanoparticles as a viable low-temperature sintering material, with promising applications in printed electronics and power semiconductors.

Keywords: copper suboxide nanoparticles, low-temperature sintering, pastes, core-shell structures, nano-micro joining

Prof. Tetsu Yonezawa received Dr.Eng. from The University of Tokyo under the supervision of Prof. Naoki Toshima. He is currently a full professor at the Department of Materials Science and Engineering at Hokkaido University. His research area is materials science and engineering, with a focus on the synthesis, characterization, and applications of metal nanoparticles in various fields, including catalysis and imaging.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-K-004)

X-ray absorption spectroscopy: The state of the art synchrotron-based characterization for energy materials

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The investigation of the local geometric and electronic structure of probing element in bulk samples is the most extensive field of application in X-ray Absorption Spectroscopy (XAS). XAS consists of two main regions which are X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS). The former region is used to explain the local geometry and oxidation states of selected element in a sample whilst the latter one is used to address the local structure around probing element in samples. In my talk, the introduction of XAS and applications of synchrotron-based XAS on advanced functional materials such as energy materials, Li-ion and K-ion battery and catalysts will be introduced in order to understand the structure and function relationship of these materials.

Keywords: X-ray absorption spectroscopy (XAS); XANES; EXAFS; energy materials

Dr. Pinit Kidkhunthod obtained a Ph.D. in Physics from the University of Bristol in 2012. He is currently a beamline scientist at the Synchrotron Light Research Institute in Thailand. His research focuses on structural studies of advanced functional materials, particularly catalysts and energy materials, using X-ray absorption spectroscopy (XAS). Since 2018, he has received continuous funding from PMU-B, PMU-C, and NRCT. He serves as an adjunct professor at the Shenzhen Institute of Advanced Technology, CAS. He has published more than 320 articles (H-index = 46) and received the Outstanding Young Materials Researcher Award from the Materials Research Society Thailand (2022).

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-K-020)

A novel reaction path-based method for chemical reaction analysis: Reaction space projector and natural reaction orbitals

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The Intrinsic Reaction Coordinate (IRC) plays a crucial role in understanding the fundamental processes of chemical reactions. In recent years, advancements in automated reaction path search methods have made it possible to discuss reaction mechanisms based on reaction path networks. By analyzing classical trajectories obtained from ab initio molecular dynamics (AIMD) simulations within these networks, it becomes possible to investigate the reaction path bifurcations and IRC jumps arising from the curvature of the IRC, thereby exploring the reaction dynamics of real molecular systems. We have developed the Reaction Space Projector (ReSPer) method, which visualizes reaction path networks in a low-dimensional space and projects AIMD trajectories onto this coordinate space. In ReSPer, classical multidimensional scaling is employed to determine principal coordinates while preserving the structural distances as much as possible between reference structures constituting the reaction path network. Additionally, we have developed the Natural Reaction Orbital (NRO) method, which visualizes electronic motion along the IRC. In the NRO method, the movement of electrons is represented as the mixing of specific occupied and virtual orbitals, which is obtained by performing singular value decomposition on the matrix of nuclear coordinate derivatives of molecular orbital coefficients along the IRC. Reaction analyses based on ReSPer and NRO provide a robust and universal approach, making them promising and powerful tools for comprehensively investigating reaction mechanisms.

Keywords: reaction path; ab initio MD; bifurcation; natural reaction orbital

Tetsuya Taketsugu (b. 1964) received his Ph.D. degree from University of Tokyo in 1994. He has been a professor at Hokkaido University since 2005 and has served as the president of the Japan Society of Theoretical Chemistry since 2023. His expertise lies in the fields of theoretical and computational chemistry, where he has made significant contributions to the development of theoretical methods for excited-state reaction dynamics and reaction path-based dynamics. He was awarded the Chemical Society of Japan Award for Creative Work in 2019 and the 15th Award of the Japan Society for Molecular Science in 2024.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-K-021)

From capture to conversion: Theoretical insights into CO_2 valorization

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The rising concentration of atmospheric CO_2 is a major contributor to climate change, demanding urgent and innovative solutions. Carbon Capture and Utilization (CCU) presents a dual benefit: mitigating CO_2 emissions while generating value-added products. In this talk, I will present our theoretical efforts toward both aspects of CCU, capture and conversion, through multiscale computational modeling. For CO_2 capture, we employ a combination of Grand Canonical Monte Carlo (GCMC), Molecular Dynamics (MD), and Density Functional Theory (DFT) simulations to investigate the performance of metal-organic frameworks (MOFs) as selective adsorbents. Our goal is to support the development of high-efficiency materials compatible with practical separation techniques such as pressure swing adsorption. Beyond capture, CO_2 electrochemical reduction offers a sustainable route to recycle CO_2 into fuels and chemicals. A key challenge in this field is promoting efficient C–C coupling to access multi-carbon (C_2+) products. We apply atomistic simulations to design and evaluate electrocatalysts, focusing on single and dual transition-metal-doped two-dimensional (2D) materials. Our findings highlight how the d-orbital occupancy and oxidation states of doped metals govern the electronic structure of catalysts, influencing their activity, intermediate binding strength, and product selectivity. By tuning these properties, we provide electrocatalysts with improved CO_2 performance.

Keywords: C_2 product; CO_2 reduction; electronic structure; C-C coupling

Supawadee Namuangruk received her Ph.D. in Chemistry from Kasetsart University in 2007. She completed her postdoctoral research at Humboldt University in Germany in 2009 before joining the Nanoscale Simulation Laboratory at NANOTEC. Her research focuses on heterogeneous catalysis, with an emphasis on periodic density functional theory and quantum chemical calculations. She was honored with the L'Oréal-UNESCO For Women in Science Award (2016) and the Wiley-CST for Green Chemistry award (2017). She is currently a Principal Researcher at NANOTEC and serves as the Chairperson of the Computational Science and Engineering Association of Thailand.

Catalytic Systems for Contemporary Challenges (S2-K-021)

Targeted design of janus particles for improved photocatalytic hydrogen evolution

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To address the global challenges of energy deficiency and environmental change, extensive research has focused on the development of renewable energy sources. As the most abundant renewable energy, solar power is a promising source to tackle the related scientific challenges. However, the intermittency of sunlight requires energy storage in the form of chemicals. In this context, hydrogen (H_2) is a clean fuel because it only produces electricity and water when used for example in fuel cells. In this context, photocatalytic water splitting for green hydrogen production has emerged as a particularly hot topic in current research, due to its low cost and environmental advantages.

In this contribution, we present the rational design of organic and inorganic semiconductor-metal Janus particles, generated by light-assisted bipolar electrodeposition. [*ChemElectroChem.* **2024**, *1*, 204; *ChemElectroChem.* **2014**, *1*, 204; *PCCP* **2020**, *22*, 22180] The resulting asymmetric nanohybrids have been tested for their photocatalytic hydrogen evolution performance and show an up to 500% higher efficiency compared to their randomly modified counterparts. Thus, this targeted Janus particle design represents a promising step forward in the frame of the development of green hydrogen production technologies.

Keywords: Janus particles; hydrogen evolution reaction; bipolar electrochemistry; photochemistry; water splitting

Alexander Kuhn is a Professor at the Institute of Molecular Science (University of Bordeaux), as well as an Adjunct Professor at VISTEC and Henan University (China). He obtained his Ph.D. from the University of Bordeaux (1994). Following postdoctoral research at Caltech, he became an Assistant Professor position (1996) and a full Professor (2000) at Bordeaux. He is a senior member of the Institut Universitaire de France, a distinguished senior member of the French Chemical Society, and a Fellow of the International Society of Electrochemistry. His current research is dedicated to electrochemistry and has been recognized by several awards, including the CNRS Science Medal in Silver (2023) and the "Grand Prix Pierre Süe" of the French Chemical Society (2024).

Catalytic Systems for Contemporary Challenges (S2-K-022)

Tackling challenges in catalysis: Surface science, in situ microscopy and waste valorization

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In the transition from fossil to renewable resources, heterogenous catalysis remains a key technology in providing chemicals, fuels, energy and a clean environment. Significant advances often follow breakthroughs in fundamental understanding or the development of new concepts. Along these lines, I discuss three recent case studies:

(i) Well-defined Ag nanoparticles, prepared by spark ablation and supported on graphite (HOPG), were characterized by various *surface spectroscopy* methods and electron microscopy. Employing an atmospheric pressure flow microreactor, the turnover frequencies (TOFs) of Ag/HOPG in ethylene hydrogenation up to 200 °C were found 200-times larger than that of unsupported Ag foil. DFT calculations indicated that H_2 adsorption was weak on unsupported Ag, whereas it increased by 0.5 eV for Ag/HOPG, driven by changes in Ag-Ag distances near the metal-carbon three phase boundary. H_2/D_2 scrambling corroborated a facilitated hydrogen activation at the metal-carbon interface, explaining its unique properties.

(ii) To directly "watch" a catalytic reaction on a metal nanoparticle, *correlative surface microscopy* was used: several techniques were applied under identical reaction conditions to the same metal nanotip (~30 nm), mimicking a *single faceted nanoparticle*. Field emission microscopy (FEM) and field ion microscopy (FIM) were employed for real-time *in situ* imaging of H_2 oxidation on a Rh nanocrystal, with and without La atom modifiers. This visualized not only the catalyst surface, but also the adsorbed reactants, so that active and inactive states could be discerned (*kinetics by imaging*), active regions identified and mechanisms elucidated.

(iii) To master contemporary challenges and reduce environmental impact, transforming hazardous and difficult-to-process waste will become crucial. We have converted spent Ni-MH batteries and aluminum waste into Ni/η-Al_2O_3 nanocatalysts for CO_2 hydrogenation with CH_4 selectivity of 99.8%. The mechanism was investigated by operando DRIFTS/GC+MS. To complete the upcycling/recycling loop, the spent Ni/η-Al_2O_3 was recycled into Ni and Al precursors.

Keywords: metal-carbon interfaces; ethylene hydrogenation; single particle catalysis; hydrogen oxidation; methanation

Günther Rupprechter (b. 1966, Ph.D. Innsbruck) is a Professor of Surface and Interface Chemistry at TU Wien, Head of the Institute of Materials Chemistry, and Director of Research of the Cluster of Excellence "Materials for Energy Conversion and Storage (MECS)" of the Austrian Science Fund (FWF). His research focuses on heterogeneous catalysis and nanomaterials, in situ (operando) spectroscopy and microscopy, and waste valorization. He has received the Jochen Block Award from the German Catalysis Society, is a member of the Austrian Academy of Sciences, a Fellow of the European Academy of Sciences, is Vice-Chair of the Austrian Catalysis Society, and has been a Guest Professor at Kasetsart University.

Catalytic Systems for Contemporary Challenges (S2-K-023)

Tailoring Nanocatalysts for CO_2 upcycling

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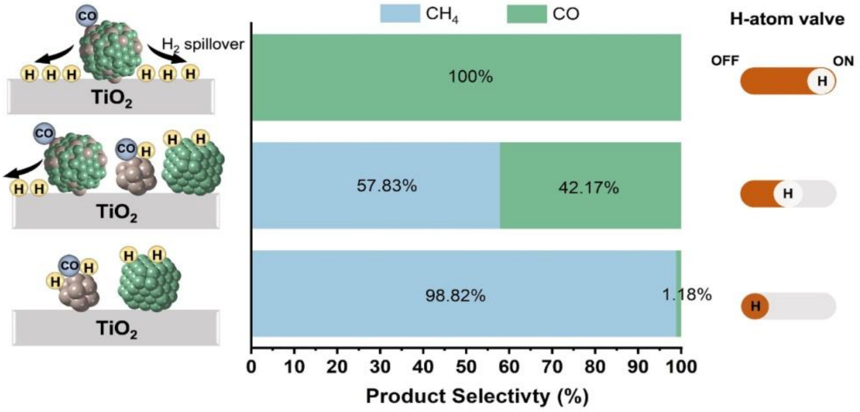
CO_2 hydrogenation to C1 chemicals has attracted significant interest due to the increasing demand of energy and global warming. Continuous efforts in the field of heterogeneous catalysis have revealed that the CO_2 hydrogenation is structure-sensitive in monometallic catalysts. However, the structure-performance relationship fundamental research in bimetallic catalysts is a big challenge because the well-defined bimetallic structures and the corresponding mechanism are more complex than monometallic ones. Here, with the construction of TiO_2 supported Ni-Ru bimetallic catalysts, evidenced by advanced microscopy characterizations, the alloyed and non-alloyed structures have been synthesised for the hydrogenation. The in-situ experiments show that the Ni-Ru bimetallic structures act like an 'H atom-valve' via controlling the H_2 spillover which can completely switch the CO_2 hydrogenation selectivity during the reaction. These findings bring a fundamentally new understanding of the selective hydrogenation on bimetallic nano-catalysis and the structure-performance relationship in controlling the 'H atom-valve' for many important chemical processes.

Keywords: nanocatalysts; CO_2 hydrogenation; CO_2 reforming of methane; structure-performance relations.



Jun Huang (b. 1977) is a Professor at the University of Sydney. He received his PhD from the University of Stuttgart (2008) and was a postdoctoral fellow at Georgia Institute of Technology and ETH Zurich. He develops emerging nanocatalysts for sustainable processes using in situ characterization techniques coupled with innovative reaction engineering. He has published over 250 articles and was awarded many prestigious awards, including the ACS Sustainable Chemistry & Engineering Lectureship Award and Australia's Most Innovative Engineer. Jun is the Editor-in-Chief of Materials Today Sustainability and the Editorial Board member of other high-ranking journals.

Catalytic Systems for Contemporary Challenges (S2-K-028)

Magnetic field-assisted, environmentally friendly catalytic CO_2 conversion to value-added chemicals for responsible chemical processes

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This study explores a novel approach to converting carbon dioxide (CO_2) into valuable chemicals using magnetic field-assisted, environmentally friendly catalysts and reaction processes. The method aims to address the urgent need for sustainable and responsible chemical processes by transforming CO_2—a major greenhouse gas—into compounds that hold economic and industrial significance. When integrated with a magnetic field, this approach enhances the efficiency and selectivity of catalytic reactions, thereby reducing energy consumption and simultaneously minimizing CO_2 emissions. Key findings demonstrate significant improvements in conversion rates and product yields, highlighting the potential for large-scale applications in the chemical industry. Moreover, this method aligns with global sustainability goals, offering a pathway to carbon neutrality while promoting the usage of CO_2 as a secondary raw material. The implications for green chemistry and industrial practices are substantial, underscoring the role of innovative technologies in advancing environmentally conscious chemical production. Through this research, we aim to contribute to the development of responsible practices that merge economic benefits with ecological responsibility.

Keywords: magnetic field; green catalysts; CO_2 conversion; responsible chemical processes; carbon neutrality

Dr. Chareonpanich earned her Ph.D. (Applied Chemistry) from Tohoku University (1996) and is currently a Professor in the Department of Chemical Engineering at Kasetsart University. Her research focuses on cleaner production, catalyst and absorbent development, VOC absorption, and green energy from greenhouse gases. She has delivered numerous keynote speeches and served as a guest editor and reviewer. Her awards include the L'Oréal Thailand "For Women in Science" Fellowship (2007), PTIT Fellow (2013–2014), Outstanding Research Awards in Material Science (2018, 2024), and the NRCT Research Group Promotion Fund (Senior Research Scholar, 2021–2024).

Catalytic Systems for Contemporary Challenges (S2-K-029)

Catalysis at interfaces: Atom-efficient metal catalysts based on single atoms, clusters and nanoparticles

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Efficient utilization of transition metals is a key requirement in the design of heterogeneous catalysts. While established design principles for nanoparticle catalysts often favor sub-optimal metal dispersion to maximize activity, metal-support interactions can critically influence performance. In particular, interfacial sites at the metal-support boundary can exhibit remarkably high reactivity.

In this talk, I will demonstrate how tailoring metal-support interfaces can significantly enhance CO_2 hydrogenation activity. Our approach combines precise synthesis of uniform active phases, operando characterization, transient kinetic studies, and DFT-based microkinetic modeling. Three case studies will be discussed: (i) Co clusters on CeO_2 and CoO/CeO_2-ZrO_2 composites, (ii) inverse CeO_{2-x}/Co catalysts for CO_2 methanation, and (iii) Cu nanoparticles confined in CIT-6 zincosilicate for methanol synthesis.

Keywords: heterogeneous catalysis; metal; CO_2; hydrogenation; structure sensitivity

Emiel J.M. Hensen b. (1971) is a professor of Inorganic Materials and Catalysis at Eindhoven University of Technology (TU/e). His research focuses on developing heterogeneous catalysts for sustainable chemical processes, including energy conversion and biomass valorization. He earned his PhD at TU/e and has since led innovative work in zeolite synthesis, catalytic mechanisms, and microkinetics. Hensen has received several prestigious grants, including Veni, Vidi, and Vici grant awards of the Dutch research council, and has published almost 700 papers. He formerly served as Dean of Chemical Engineering and Chemistry at TU/e and chairs the Netherlands Institute for Catalysis Research (NIOK).

Advanced Coordination Materials and Catalysis for Environment (S3-K-001)

Redox-neutral approaches to organophosphinates: Cross-metathesis and phosphate activation strategies

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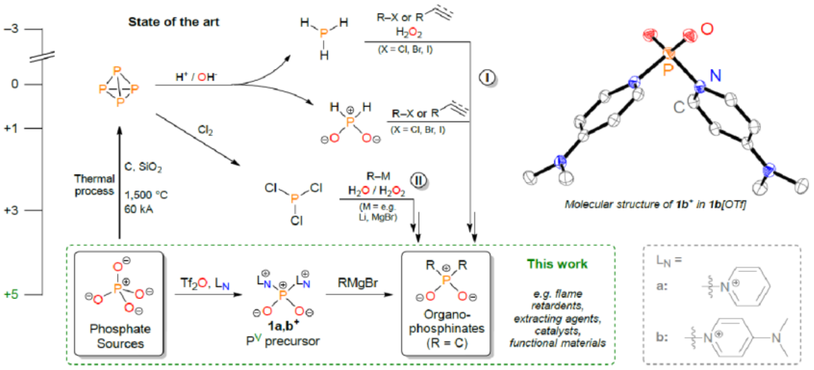
Organophosphinates ($R_2P(O)OR'$) are versatile compounds with applications in catalysis, materials chemistry, extraction processes, and as bio-relevant functional groups. However, their conventional synthesis relies heavily on white phosphorus (P_4), posing significant environmental and safety concerns due to its pyrophoricity and energy-intensive production. To address these challenges, we have developed a redox-neutral activation strategy for phosphates using electrophilic phosphorylation reagents, enabling the direct synthesis of diaryl- and dialkynylphosphinates without P_4 intermediates. This approach, based on the use of tailored leaving groups such as 4-dimethylaminopyridine (DMAP), facilitates highly selective phosphorylation of nucleophiles, significantly expanding the synthetic scope.

As a complementary strategy, we explored the reactivity of alkenyl-substituted phosphates in ruthenium-catalyzed cross-metathesis reactions, providing insights into the role of phosphate substituents in controlling metathesis selectivity. Notably, while allyl and butenyl phosphates underwent productive metathesis, vinyl phosphates led to the unexpected formation of a ruthenium carbide complex, shedding light on mechanistic aspects of the reaction. These findings demonstrate the potential of phosphate-based substrates in catalytic transformations and contribute to the development of sustainable phosphorus chemistry.

Keywords: redox-neutral phosphate activation; sustainable phosphorus chemistry; cross-metathesis of phosphates; organophosphinate synthesis; electrophilic phosphorylation



Prof. Jan J. Weigand (1974) studied chemistry at LMU Munich, earning his Dr. rer. nat. in 2005 with distinction. He was awarded the Bavarian Culture Prize and later received a Lynen Scholarship (AvH Foundation) for postdoctoral research at Dalhousie University, Canada. After habilitation at WWU Münster (2007), he secured a Liebig Scholarship (FCI) and an Emmy Noether Fellowship (DFG). He joined TU Dresden as a professor in 2013, focusing on sustainable phosphorus chemistry, technical applications, and recycling. Recognized with an ERC Starting Grant (2012) and DFG Reinhart Koselleck funding (2023), his work advances circular economy strategies in chemistry.

Advanced Coordination Materials and Catalysis for Environment (S3-K-008)

Catalysis for the environment: Sustainability for the chemical industry

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Chemical industry currently focusses on an increase of the sustainability of their production. One key factor in this effort is catalysis, here typically both heterogeneous and homogeneous catalysis, the latter using coordination compounds, are explored.

The presentation will address recent contributions of homogeneous catalysis to a number of production problems. These studies were conducted in the Catalysis Research Laboratory (CaRLa), [*J. Org. Chem.* **2019**, *84*, 4604–4614] a common industry-on-campus laboratory of BASF SE and Heidelberg University:

a) high catalytic activity in order to use low catalyst loadings
b) the use of carbon dioxide as a building block for polymers
c) new polymerization catalysts
d) de-polymerization catalysis

The presentation will include structural details of the catalysts, mechanistic experiments and accompaning computational studies. Also the improvement of the environmental impact for the production process will be discussed.

Keywords: homogeneous catalysis; transition metals; industrial research; mechanisms; computational studies

Born 1963, Ph.D. from LMU Munich (1991) with G. Szeimies. Postdoc with B.M. Trost at Stanford (1991-1993). Assistant Professor with J. Mulzer at Free University of Berlin, University of Frankfurt and University of Vienna. Visiting Scientist at the University of Tasmania (1999). Temporary Professorship at Marburg University (1999), Associate Professor at Stuttgart University (Associate Professor, 2001), Full Professor at Heidelberg University since 2007. Dr. Otto Röhm Memorial Fellowship (1998); Karl-Ziegler Memorial Fellowship (2001), ORCHEM Prize for natural sciences of the German Chemical Society (2002); Hector Research Prize 2010.

AI in Drug Discovery Research (S5-K-004)

Developing new methods for drug design and repositioning

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Drug design (CADD and AIDD) has been facing a long-term and fundamental challenge of predicting the binding between the structurally ever-changing proteins and ligands, let alone so called induced-fit interaction during the binding process. This talk will present my work of developing new methods for overcoming the challenge and their application in new drug discovering and old drug delocalization, including: developing enhanced MD sampling methods, e.g. vsREMD, that could significantly increase the MD simulation efficiency for sampling the protein conformation change; developing method to quantitatively describe the dynamic behavior of ligand binding pockets of target proteins, namely D3Pockets, based on the MD simulation results; developing multifunctional platform, namely D3CARP, for target prediction and virtual screening; application of the newly developed method in discovering the new ligands and drug repositioning.

Keywords: drug design; new methods; molecular dynamics, drug repositioning

Prof Weiliang Zhu, born in 1963, obtained his PhD from Shanghai Institute of Materia Medica (SIMM), the Chinese Academy of Sciences (CAS) in 1998. He is currently working as professor and principal investigator in Shanghai Institute of Materia Medica (SIMM) CAS, and as head of drug discovery design center at SIMM since 2009. The main research area in Prof Zhu's lab is CADD, especially, focusing on the development of new methods and theories, as well as the application of new methods. Currently, the target proteins under study in the lab are mostly related to diabetes, cancer and infectious diseases.

AI in Drug Discovery Research (S5-K-007)

Revolutionizing drug discovery: The transformative power of AI in therapeutics

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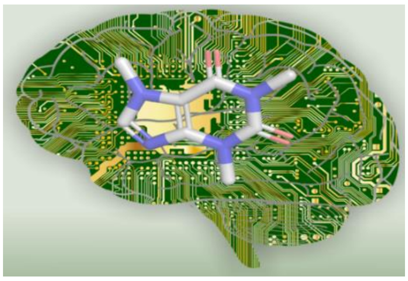
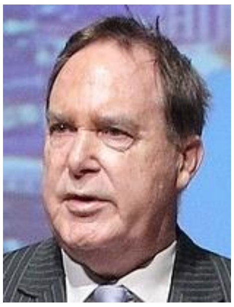
We are currently witnessing paradigm shifting scientific developments. The almost infinite number of accessible materials provide an inexhaustible supply of potential drugs and materials with valuable properties if we can find them. This has driven a rise in rapid automation for synthesis of molecules and measurement of properties, generating databases of complex genetic, structural, chemical, property, and biological information.

Finding 'islands of chemical utility' in vast spaces has also driven development of machine learning methods (ML), like deep learning and large language models. ML algorithms are universal approximators, prompting an unprecedented rise in applications to many aspects of life – medicine, finance, manufacturing, social media etc. In chemistry, we now have rapid and accurate quantum machine learning methods, generative methods that use models that suggest new molecules with improved properties, accurate prediction of protein structures from sequence, nascent general AI in ChatGPT, vast 'make on demand' chemical libraries, emerging autonomous chemical discovery systems (self-driving labs), and use of evolutionary AI methods for discovery.

This paper discusses the drivers for these developments and exemplifies how my collaborators and I use ML in biomaterials and regenerative medicine, drug design of drugs, biologics, and vaccines, and cancer diagnostics.

Keywords: machine learning; drug and biomaterials design; artificial intelligence, biologics and vaccines





David Winkler is Professor of Biochemistry and Chemistry at La Trobe University, Professor of Pharmacy at the University of Nottingham, and Professor of Medicinal Chemistry at Monash University. He applies computational chemistry, AI, and machine learning to the design of drugs, agrochemicals, electrooptic materials, nanomaterials, green corrosion inhibitors, catalysts, and biomaterials. His is a recipient of an ACS Skolnik award, a Royal Australian Chemical Institute Distinguished Fellowship, and the AMMA Medal. He has written >300 journal articles and book chapters (6 ISI Highly Cited) and is an inventor on 25 patents.

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-K-013)

The role of natural and organic ingredients as emerging nutrition trends

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The role of natural and organic ingredients as emerging nutrition trends. Let's start by recalling the previous interactions. They've been exploring challenges and opportunities related to sourcing, cost, regulations, and international trade variations. Now, they want to know how these ingredients fit into current nutrition trends. First, to define what natural and organic mean in the context of nutrition. Natural typically refers to minimally processed, no artificial additives, while organic involves specific farming practices without synthetic chemicals. Both are gaining traction due to health and environmental concerns. Next, should consider why these are emerging trends. Health-conscious consumers are driving demand, but also sustainability plays a role. People are more aware of how their food choices impact the environment. There's also the aspect of clean labels—consumers want transparency. Then need to break down the role into key points. Maybe start with consumer demand factors: health benefits, clean eating, sustainability. Then look at the impact on the food industry: product innovation, reformulation, certifications. Also, address challenges like cost and accessibility, which were mentioned before but in the context of nutrition trends. Opportunities here would include market growth, functional foods, and partnerships. But challenges might be greenwashing, regulatory inconsistencies, and supply chain issues as a challenge for global nutrition trends. Then should also think about how these ingredients contribute to specific dietary trends, like plant-based diets or gut health. Probiotics, prebiotics from natural sources, organic superfoods—those are relevant. Including examples like quinoa, chia seeds, or organic fermented foods could illustrate the points. And try to mention the role of certifications in building trust. USDA Organic, Non-GMO Project Verified, Bio Label etc., help consumers identify genuine products. However, there's the issue of multiple standards across regions, which can confuse consumers and complicate trade. Education is another aspect. Consumers need to understand the benefits of natural and organic ingredients to justify higher prices. Brands that educate through marketing or labeling can build loyalty. In conclusion, the role is multifaceted, influencing consumer choices, industry practices, and even agricultural methods. The answer should highlight how these trends are shaping the future of nutrition, balancing health, sustainability, and economic factors.

Keywords: natural and organic ingredients; nutrition trends; education

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-K-014)

Buying health on the shelf: New life-changing healthy products in stores 2025

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The Healthy Product Trends of 2025 those are revolutionizing Healthcare at reach. The year 2025 is poised to be a pivotal moment of transformative changes in self-healthcare. Groundbreaking technological advancements will reshape everyday consumer products, enhancing efficiency and availability. 5 big health challenges these people of the 21st century are facing with, and they are needed to be addressed in day-by-day living. What a truly remarkable to put the everyday solutions on the grocery's shelfs, those people can grab and go to maximize health and protect themselves from going under.

1. Nutritional Deficiency is still a health problem to general public. Even we are at the point of living in abundant, but the way many choice to consume and other factors are the biggest things to take a toll on many of us. Products are not only easy to get and taste good, but also, have to be nutritious enough for us to thrive on.
2. Mental health nutrients play a crucial role in supporting individuals struggling with stress, anxiety, post-traumatic stress disorder (PTSD), and other everyday mental health challenges. Foods and drinks to go offer accessible, self-care, allowing individuals to receive substances to help to ease up mental conditions from virtually anywhere and encouraging them to realize what to consume to change their state of being.
3. The gut microbiome is a critical factor for overall health, influencing digestion to mental well-well-being. In 2025, microbiome research is expected to grow significantly, with scientists gaining a deeper understanding of how these microbial communities affect human health, helping to develop more sophisticated and effective probiotics and prebiotics which surely put in a form of products that can be bought from the shelf easily.
4. Sight Degeneration which happens in all ages and sexes. We are bombarding mass information into us every single day in a big quantity. Most of our information comes in the form of digitalization where visual consumption is involved. Aged related degeneration is progressing as we get older, but a new form of degeneration on top of this is visual degeneration from light rays that we get from electronic devices and sun exposures. Protecting our eyes and slowing down the degeneration becoming an everyday effort no one should ignore.
5. Genomic research is unlocking new avenues of understanding in human biology, providing foundational genetic insights, and enhancing our knowledge of the mechanisms underlying various diseases, particularly genetic disorders and cancers. Genetic data can help healthcare professionals devise appropriate and general race. according to the unique genetic profiles of the pack.

The health trends anticipated for 2025 signal a significant transformation of the healthcare landscape. Products will become increasingly precise and personalized, emphasizing holistic care that addresses physical and mental well-being driven by cutting-edge technology. The year 2025 will revolutionize healthcare, ushering in a new era of precision and accessibility that promotes sustainable and improved well-being.

Keywords: health; shelf; health products market trend

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-K-015)

Nano-enhanced nutraceuticals: Pioneering solutions for next-generation preventive healthcare

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The integration of nanotechnology with nutraceutical science is revolutionizing how bioactive compounds are delivered, absorbed, and utilized in the body, offering unprecedented potential for disease prevention and health optimization in Asia. This presentation emphasizes the latest progress in nanoformulations including nanostructured lipid carriers, nanoemulsions and polymeric nanoparticles, that improve the stability, bioavailability, and targeted delivery of nutraceuticals such as polymethoxyflavones (*Kaempferia parviflora*), resveratrol, and omega-3 fatty acids. With Asia facing a surge in lifestyle-related diseases, these innovations provide scalable, culturally adaptable strategies to combat diabetes, cardiovascular disorders, and immune deficiencies. The discussion will also address critical challenges, including regulatory harmonization, safety assessments, and sustainable production, while showcasing successful case studies from the region. By bridging traditional knowledge with cutting-edge nanotechnology, this session will chart a roadmap for the future of preventive healthcare, emphasizing interdisciplinary collaboration to meet Asia's unique nutritional and medical needs.

Keywords: nanotechnology; nutraceuticals; bioavailability; controlled delivery; traditional medicine; market opportunities; economic growth

Green Chemistry; Paving the Way to a Sustainable Future (S8-K-002)

Sustainability based on green chemistry of novel domino reactions

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Nitesh K. Gupta, Mohit Kapoor, Shwu-Chen Tsay
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Sustainable chemistry is a scientific approach aimed at optimization of the use of natural resources to meet human needs for chemical products while minimizing environmental impact. Green chemistry, as discussed here, focuses on the design, synthesis, and application of chemicals through various domino processes that reduce pollution and environmental risks. It establishes the core principles of sustainable science and ensures ecologically responsible development. Our contributions highlight the importance of key processes in advancing a sustainable future. This talk comprises three topics: the development of *a new reaction*, the invention of *a novel chemical reagent*, and an *innovative application of a commonly used solvent*. Topics are Generation of Quaternary Carbons in Cycloalkanones and Lactones with Arynes through a Domino Process, Calcium-Impregnated Silica Gel in a Domino Reaction Involving *Irreversible* Aldol Addition, Dehydration, and Michael Addition, and Sustainable Domino C–N/C–C Bond Formations by Use of Acetonitrile in a Solvent-Free Reaction with Outstanding *E*-Factors and High Volume Productivity. These three independent multistep reactions, carried out in a single flask, align with the principles of green chemistry by minimization of the use of hazardous substances and reduction of waste. Our newly developed domino reactions address fundamental chemical challenges while promoting sustainability. The outcomes enable efficient production of valuable compounds with lower environmental impact, and thus enhance profitability.

Keywords: quaternary carbons; Ca-SiO_2; solvent-free reaction; domino reaction

Reuben Jih-Ru Hwu: born 1954, National Taiwan University (B.S. 1976); Stanford University (Ph.D. 1982); Distinguished Chair Professor Emeritus of Lifetime Honor (2024–). Research fields: organic synthesis, organosilicon chemistry, and nano-biomaterials. President of the Federation of Asian Chemical Societies (2019–23), Fellow of The Academy of Sciences for the Developing World (1999–), Fellow of IUPAC (2000–), Fellow of The Royal Society of Chemistry (2005–), Fellow of The Federation of Asian Medicinal Chemistry (2005–), Member of the European Academy of Sciences and Arts (2019–).

Young Career Development under FACS-ACS Collaboration (SA-K-001)

Adding value to Asia chemistry: Reflections on forty years of research, networking and mentorship

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My first research trip to Asia was in January 1985 when I visited Bangkok (Ramkhamhaeng University) and three universities in Manila. Scientists in both countries were beginning to recognize the value of their marine resources and sought collaborative opportunities for research training and access to instrumentation for data acquisition. There was funding support from UNESCO and from Australian government agencies. Since then, I have had the privilege of interacting with young scientists in several Asian countries, some students bringing samples under permit for analysis, others with scholarships to undertake postgraduate research in my laboratory. There has been a focus on alkaloids from Asian medicinal plants such as *Pandanus* spp. as well as terpenes and peptides from marine samples.This talk will describe some scientific highlights of these research interactions. In addition, the shared benefits of mentoring and networking with Asian colleagues have facilitated my contributions to international events such as the annual Global Women’s Breakfast of IUPAC.

Keywords: biodiversity, natural products, alkaloid, terpene, peptide, NMR

Mary Garson is Professor Emerita at the University of Queensland in Brisbane. She completed her PhD at the University of Cambridge in 1977, and then held research or academic positions in Rome, Townsville, and Wollongong. She is a Fellow of the Australian Academy of Science and President-Elect of the International Union of Pure and Applied Chemistry. In 2019, she became a Member of the Order of Australia for her significant service to education.

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-K-017)

Scientific insights into indigenous formulations: A pathway to natural therapies for obesity, diabetes, hypertension, and oxidative stress

Poornima Jeewanthi,[1] Dinum Perera,[2] Nimanthi Jayathilleke,[1] Kapila Senevirathne,[1]
Renuka Attanayake,[3] Priyani Paranagama[1,*]
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[2] *Department of Bioprocess Technology, Faculty of Technology,*
Rajarata University of Sri Lanka, Mihintale, Sri Lanka
[3] *Department of Plant and Molecular Biology, Faculty of Science, University of*
Kelaniya, Kelaniya, Sri Lanka
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Traditional medicine has long been integral to healthcare, especially in regions rich in indigenous knowledge. Sri Lanka, with its abundance of medicinal plants, offers a vast source of bioactive compounds for therapeutic use. However, many traditional remedies lack systematic scientific validation. This keynote address explores the bioactivity of indigenous herbal formulations, particularly in managing obesity, diabetes, hypertension, and oxidative stress.

Our research combines ethnopharmacological knowledge with modern methodologies to assess the efficacy of polyherbal formulations. *In vitro* and *in vivo* studies have evaluated key biochemical markers, enzyme inhibitory activities, and mechanistic pathways. Notably, bioassays reveal anti-obesity effects via pancreatic lipase inhibition and antihyperglycemic activity through α-amylase and α-glucosidase inhibition. Antihypertensive properties have been demonstrated via ACE inhibition, while antioxidant potential has been confirmed using DPPH, FRAP, TBARS and ABTS assays.

Advanced chromatographic techniques have identified active phytochemicals responsible for these effects. Insights from animal models and clinical observations further support their efficacy and safety. This presentation highlights the need for systematic research to validate and optimize indigenous formulations, fostering evidence-based, plant-derived medicines for metabolic disorders and oxidative stress.

Keywords: indigenous medicine; antihypertension; antihyperglycemic; antioxidant; antiobesity

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-K-018)

Plants as the source of renewable chemicals for a sustainable society: Applications in advanced functional material, drug delivery and cancer therapy

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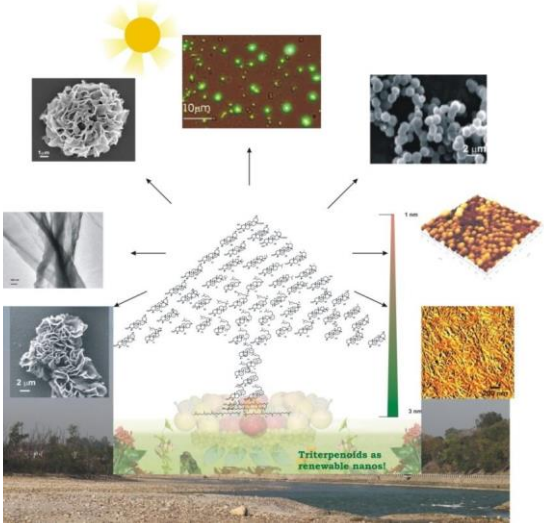
Plant metabolites are highly promising renewable alternative to fossil and petroleum resources for a sustainable future. Among various plant secondary metabolites, terpenoids constitute the most numerous and structurally diverse group of natural products. Isolation of over 55,000 terpenoids have been reported until recently and the number has been increasing steadily. Utilization of the plant metabolites in various areas of science, technology and society is of tremendous importance to combat global depletion of fossil fuels. We have reported that all the terpenoids are of nanometer long having varied rigid and flexible lengths. The di- and tri-terpenoids and apo-carotenoids isolated from plants such as crotocembraneic, arjunolic, betulinic, oleanolic, glycyrrhetinic and ursolic acids, betulin and bixin self-assembled in liquids at low concentrations affording self-assembled nano- to micro-sized architectures such as helical fibers, vesicles, spheres, and gels. The self-assemblies were capable entrapping fluorophores including the anticancer drug doxorubicin. [*Pure & Appl. Chem.* **2020**, *92*, 567–577] A novel organic-inorganic hybrid material generated from arjunolic acid and in-situ generated Pd-nano particle acted as a recyclable catalyst for C-C coupling reactions and reduction reactions. In-vitro studies revealed selective cytotoxicity of sodium maslinate in leukemic cell. An apocarotenoid bixin self-assembled spontaneously in aqueous organic liquids yielding vesicles capable of entrapping anticancer drugs. [*Chem. Asian J.* **2024**, *19*, e202400361] Recent results will be presented in the perspective of green, renewable and nanos.

Keywords: plant secondary metabolites; terpenoids; self-assembly; vesicles; drug-delivery



Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-K-019)

Environmental toxins and heavy metal exposure: Unraveling risk factors for chronic kidney disease of unknown etiology (CKDu) in endemic regions

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Chronic Kidney Disease of unknown etiology (CKDu) has become a major public health concern in several regions worldwide, including Sri Lanka, with rural agricultural communities being disproportionately affected. The potential role of environmental toxins, including heavy metals and trace elements, as risk factors for CKDu has been extensively studied. Research in CKDu-endemic regions, such as the North Central, Central, and Uva provinces, has identified the presence of toxic metals like lead (Pb), arsenic (As), cadmium (Cd), and chromium (Cr) in paddy soils, groundwater, and staple foods. While these metals often remain within permissible limits, their gradual accumulation in agricultural ecosystems poses a long-term threat. Paddy soils in high-risk areas exhibit elevated levels of toxic metals, with potential translocation into rice plants, a dietary staple. Groundwater in these regions, though largely compliant with safety standards, occasionally contains excessive fluoride and anionic species, raising concerns about chronic exposure. Dietary exposure to toxic metals further exacerbates the risk. Studies highlight certain foods, including rice, leafy vegetables, and inland fish, contain Pb levels exceeding safety thresholds. Hierarchical analysis suggests a common source of Pb accumulation, and hierarchical clustering reveals an intricate connection between As and Cd, indicating a potential common origin. While individual concentrations comply with acceptable standards, the synergistic effects of Cd and As accumulation might pose elevated health risks. Although heavy metals in water, sediment, and soil do not directly correlate with CKDu prevalence in some regions, their cumulative impact, combined with other environmental and lifestyle factors, underscores the need for comprehensive risk assessments. Addressing environmental toxins through targeted interventions, sustainable agricultural practices, and continuous monitoring is critical to mitigating CKDu risks and safeguarding public health.

Keywords: bioaccumulation; chronic kidney disease of unknown etiology (CKDu); environmental toxins; heavy metals; synergistic effects

Sustainable Chemistry for Agricultural Residue Valorization (SG-K-005)

Lignin valorization: From academic findings to commercializations

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Future products need to meet current demands in terms of properties: and be produced from renewable resources. From environmental sustainable perspectives, low value side streams that currently are burnt should be prioritized. Kraft pulping gives a pulp of high value and a stream that generates energy while recovering the process chemicals. The recovery of process chemicals in the recovery boiler is the bottleneck of the pulping process. A way to increase pulp production is by debottlenecking the recovery boiler by removing some of the lignin. The cost of removing the lignin does not compensate the increased revenue from pulp production alone: and a value of lignin above its heating value is required.

In this talk, a few examples of value chains from Kraft lignin will be presented, disclosing challenges and opportunities of using Kraft lignin as a raw material in the production of biofuels, thermoplastics and thermoset materials. The production of said materials will be discussed in economic and environmental perspectives.

Keywords: pulping; lignin; biofuel, biomaterials; life cycle assessment

Dr. Joseph S.M. Samec earned his Ph.D. in 2005 from Stockholm University under Prof. Jan-E. Bäckvall. He completed a postdoc with Robert H. Grubbs at Caltech (2006–2007) and worked as Research manager at OrganoClick (2008–2009). He began an independent research career at Uppsala University and returned to Stockholm University in 2015. In 2021, he took a sabbatical at University of Padova to learn life cycle assessment. His research focuses on sustainable chemistry and he has co-founded spin-off companies like RenFuel and LigniCore, which utilize lignin from the forestry industry.

INVITED ABSTRACTS

Analytical Chemistry (AC-I-044)

Electrochemical paper-based analytical devices for the determination of nitrite, nitrate and nitrosamine

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Nitrite and nitrate are widely employed in the food industry to enhance color, texture, and shelf life. However, their presence—whether added directly or formed via bacterial reduction—can pose significant health risks, including methemoglobinemia and carcinogenesis through the formation of N-nitrosamines. Consequently, reliable multiplex detection methods are urgently needed. This study presents an innovative, manually rotated paper-based analytical device (PAD) featuring a horizontal, "yoyo-like" design that mimics centrifugal mixing, enabling the simultaneous detection of nitrite and nitrate. Nitrite is measured directly, whereas nitrate is quantified via its electrochemical response following reduction to nitrite using zinc dust. The rotational mechanism enhances mixing and ensures uniform reagent contact, thereby improving detection efficiency. To broaden the platform's capabilities, we developed electrochemical PADs (ePADs) capable of detecting nitrite, nitrate, and N-nitrosamines through three distinct sensing strategies integrated into a single device. These portable, low-cost sensors provide a user-friendly approach for on-site analysis. Application to real meat samples demonstrates the method's practicality, accuracy, and strong potential for food safety monitoring.

Keywords: electrochemical sensor; multiplexed detection; nitrite; nitrate; nitrosamine

Anchalee Samphao is an Associate Professor of Analytical Chemistry, specializing in electrochemical sensors and biosensors. Her research focuses on paper-based sensors for detecting food contaminants, pathogens, and environmental pollutants, integrating advanced materials like MOFs and nanocomposites. She has led several nationally funded projects and published widely in high-impact journals, with a strong emphasis on developing practical, low-cost diagnostic technologies.

Analytical Chemistry (AC-I-046)

γ-Hydroxybutyric acid detection using a colorimetric sensor and graphene field-effect transistor (GFET) sensor

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γ-Hydroxybutyrate (GHB), known as a date rape drug, induces symptoms like amnesia, confusion, ataxia, and unconsciousness when mixed into drinks and ingested by an unsuspecting individual. To address the challenges of promptly and discreetly detecting GHB in beverages, we have developed a portable colorimetric and graphene field-effect transistor (GFET) sensors. This colorimetric sensor utilizes a colorimetric sensor fabricated with polyvinyl alcohol (PVA), polyurethane (PU), and polyacrylonitrile (PAN) nanofibers (NFs), integrated with the chemical receptor 2-(3-bromo-4-hydroxystyryl)-3-ethylbenzothiazol-3-ium iodide (BHEI). The second skin, comprising PAN conjugated with BHEI NFs (PB NFs), offers simplicity, high sensitivity, and rapid color change. The second skin platform effectively detects GHB at concentrations as low as 0.01 mg/mL, achieving detection within 50 seconds for both 1 and 0.1 mg/mL GHB solutions when applied to fingertips or wrists. It suitable for discreet real-life use, empowering individuals to protect themselves from drug-facilitated sexual assault crimes anytime and anywhere. In addition, we developed a biosensor based on a graphene field-effect transistor (GFET) functionalized with GHB receptors for highly sensitive and rapid detection of externally exposed GHB solutions and clinical samples containing exogenous GHB.

Keywords: γ-hydroxybutyrate; date rape drug; colorimetric sensor; FET sensor

Oh Seok Kwon received his Ph.D. in Chemical and Biological Engineering from Seoul National University in 2013. He began his academic career at Sungkyunkwan University, where he currently holds the position of Associate Professor at the SKKU Advanced Institute of Nanotechnology and the Department of Nano Engineering. His research interests focus on the development of graphene-based field-effect transistor (GFET) sensors, drug sensors, and bioelectronic systems for ultra-sensitive chemical and biological detection. He has published in leading journals including Advanced Functional Materials, Advanced Materials, and ACS Nano, and serves as a Guest Editor for Sensors and an Editorial Board Member for Polymers.

Analytical Chemistry (AC-I-047)

Non-enzymatic detection of glucose, and glucose-ketone ratio (GKR) via formation of silver nanoparticles and iron-acetate complexes on paper-based analytical devices

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The World Health Organization (WHO) has established seven guidelines for the development of a diagnostic tool: Affordable, Sensitive, Specific, User-friendly, Rapid and Robust, Equipment-free, and Delivered to those who need it (ASSURED). This necessitates the utilization of simple point-of-care testing (POCT) for the detection of diseases that the general public can utilize. This requirement can be met through the implementation of paper-based analytical devices (PADs). This promising analytical platform encompasses a combination of portability, ease of use, low cost, and reliability for the rapid detection of diseases. In this work, we will discuss the rapid detection of diabetes mellitus by employing silver nanoparticles and in-situ synthesis of nanoparticles on the PADs for quantitative/semiquantitative glucose, glucose-ketone ratio (GKR) detections in urine samples. The devices are capable of detecting non-enzymatic glucose and ketone levels. Glucose is assessed through the synthesis of silver nanoparticles (AgNPs) stabilized by various floral honey types. Ketone is measured via the formation of an iron-acetate complex. This study further investigates the efficacy of different floral honey types as capping agents for AgNPs formation, with the objective of enhancing the accuracy and reproducibility of glucose ketone ratio (GKR) detection. AgNPs are characterized ATR-FTIR spectroscopy and UV-Vis spectrophotometry. ImageJ is employed to quantify colorimetric reaction distances on the PADs. Optimized parameters identified rambutan honey as the most effective capping agent for GKR detection on the PADs. The optimal conditions for this method include a 10% (v/v) honey concentration, 60 mM silver nitrate, 1 M glycine in pH 9.4 phosphate buffer, and a 15-minute reaction time. The validation of this method demonstrated excellent linearity ($R^2 = 0.9971$), high precision (RSD = 2.85%), and accuracy (93.40 - 99.83%). The limits of detection and quantification were determined to be 12.05 and 40.17 mM/dM, respectively.

Keywords: glucose; ketone; paper-based devices; nanoparticles; disease

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Analytical Chemistry (AC-I-048)

New strategies for electrochemical detection of cancer biomarkers

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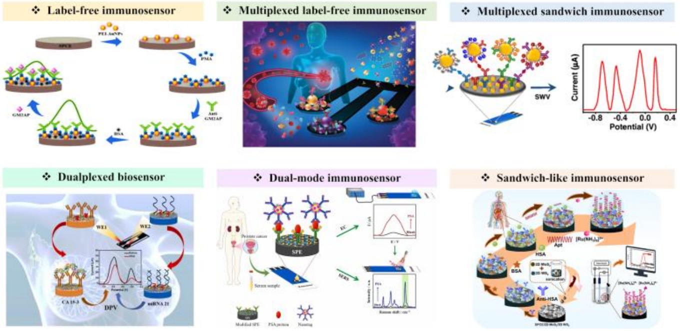
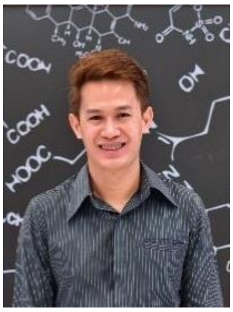
The power of ultratrace-level quantitative assays for disease protein biomarkers holds great potential. By detecting diseases at their earliest, most treatable stages, these assays help clinicians diagnose with unparalleled accuracy. They also provide researchers with insights into the body's responses to diseases and treatments, facilitating a better understanding of achieving in-body restorations. Electrochemical biosensors prove effective in detecting such biomarkers and possess good analytical performance. Their advancements rely on integrating functional nanomaterials using various fabrication and detection strategies to enhance sensitivity and specificity. Incorporating novel state-of-the-art nanomaterials, such as nanoparticles, quantum dots, and two-dimensional nanomaterials, each with unique characteristics, has further propelled these developments. At Chiang Mai University, our research focuses on constructing innovative biosensors with new configurations. These sensors, developed by our team, have the unique capability to detect both single and multiple target biomarkers. The responses from the amplification strategies due to the formation of the target-receptor complexes exhibit a proportional relationship to the targets' concentrations. Our sensors exhibit outstanding sensitivity, selectivity, reproducibility, and stability, achieving low detection limits suitable for identifying disease biomarkers at clinically relevant cut-off levels. The success of our work suggests the potential for practical applications in the field of clinical diagnoses.

Keywords: electrochemical sensor; biomarker; disease; nanomaterial





Kontad Ounnunkad is an associate professor in the Department of Chemistry at Chiang Mai University, Thailand. He received his Ph.D. in Chemistry from the University of Wollongong, Australia, in 2010. At Chiang Mai University, his research focuses on developing new electrochemical sensors for clinical diagnoses of noncommunicable diseases (NCDs) and infectious diseases. He has also developed 2D materials for electrochemical devices, especially energy storage. He was recently on the list of the World's Top 2% Scientists 2022/2023/2024 in Applied Physics and Analytical Chemistry by Stanford University/Elsevier.

Analytical Chemistry (AC-I-049)

Hyperspectral near-infrared measurements for sensitivity enhancement in analyzing thin sheet samples and identification of pearls with different cultured origins

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A diffuser-supported hyperspectral near-infrared (DS-HS-NIR) measurement scheme in which a Teflon plate as a photon diffuser was placed beneath a thin sheet sample for trans-reflectance spectral acquisition was proposed to enhance peak intensity (sensitivity) of the sample. The scheme was to increase the number of sample-interacting photons by generating diffused photons using a Teflon (diffuser) and directing them toward a spectroscopic sampling area to additionally interact with a sample, increasing the intensity of the subsequent peak. When the weighing paper, plastic gloves, and mesh fabric sheets (thickness: 20–230 μm) were measured using a conventional scheme without using the diffuser, peaks corresponding to the sheet samples were difficult to recognize; with the diffuser, they were apparent with enhanced intensity. Further, the increased number of sample-interacting photons when using the diffuser was confirmed by Monte Carlo simulation. Also, hyperspectral imaging near-infrared (HSI-NIR) spectroscopy was exploited to discriminate (i) beaded salt water-cultured (B-SW), (ii) beaded fresh water-cultured (B-FW), (iii) non-beaded fresh water-cultured (NB-FW), and (iv) imitation pearls. The distinction of B-SW, B-FW, and NB-FW pearls was feasible since their NIR spectra were dissimilar depending on the characteristics of pearls such as chemical composition, irradiance (orient), and gloss.

Keywords: hyperspectral imaging near-infrared spectroscopy; thin polymer sheet; dried laver sheet; pearl evaluation; cultured origin

Hoeil Chung is a Professor of Chemistry at Hanyang University, Seoul. He received his Ph.D. from the University of Iowa in 1994 and worked at SK Energy before joining Hanyang in 2002. His research focuses on Raman and NIR spectroscopy, SERS-based biomarker detection, and metal-alloy nanostructures. He has published over 200 peer-reviewed papers.

Analytical Chemistry (AC-I-050)

Micromotors meet collective biosensing

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Micromotors are microscale devices with enormous potential for analytical (bio)-sensing due to their collective autonomous motion capabilities in extremely low amounts of samples or for guided detection in localized hard-to-reach areas. Such unique features allow for dynamic interactions with the analytes holding considerable promise in microscale environments and opening new avenues for on the fly (bio)-sensing strategies. In our lab, we are focusing on the design and development of tubular and Janus micromotors that confer them self-propulsion using (photo)-catalytic propulsion and magnetic guidance with compatibility in biological media. They also smartly incorporate nanomaterials and molecular recognition-based functionalization to obtain sensitivity and exquisite selectivity on board using optical and electrochemical detection approaches, even integrated on smartphones or as smart SERS substrates. Micromotor technology has become an attractive alternative to performing fast, and reliable bioassays and diagnostic testing, especially when an extremely low volume of samples is available or when the analysis must be performed in a micro-size environment.

Keywords: mobile biosensors; fluorescence; electrochemical; controlled motion

Alberto Escarpa is a Full Professor of Analytical Chemistry at the University of Alcalá. His research focuses on analytical microfluidics and micromotors. He has published over 200 papers, delivered numerous invited lectures, and has been recognized among the world's top 2% most cited scientists. His work has featured on journal covers such as Angewandte Chemie and Chemical Science. He received the 2024 Spanish Royal Society of Chemistry Award for Research Excellence and currently serves as Editor-in-Chief of Microchimica Acta and on the Editorial Advisory Board of Analytical Chemistry.

Analytical Chemistry (AC-I-051)

Electrochemical biosensors for rapid detection in HCV quantification and cancer status determination

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We demonstrate novel electrochemical biosensors for infectious disease diagnostics, combining DNA detection techniques with molecular assays for biomedical applications. Our approach employs gold nanoparticle-labeled DNA strand displacement strategies on electrochemical platforms, achieving direct detection of hepatitis C virus (HCV) RNA in clinical plasma without extraction or amplification. The system delivers highly sensitivity (4 fM for synthetic targets, 43 ng/μL for RT-PCR products) with results matching conventional RT-PCR in clinical samples. We have extended this technology to monitor viral DNA physical status changes in cancer progression using differential pulse voltammetry. Key advantages include rapid testing (30 minutes), minimized sample handling, reduced contamination risk, and field adaptability with lyophilized reagents stable for 90 days at 4°C. The platform's versatility is demonstrated through variation to other tropical diseases, including a high-specificity aptasensor for leptospirosis targeting electron transfer flavoprotein beta. These innovations advance point-of-care diagnostics for resource-limited settings, supporting global disease control efforts.

Keywords: electrochemical biosensor; DNA strand displacement; gold nanoparticles; hepatitis C virus; cancer biomarkers

Benchaporn Lertanantawong is an Associate Professor of Biomedical Engineering at Mahidol University. She received her Ph.D. in Biotechnology from King Mongkut's University of Technology Thonburi. Her research focuses on nanobiosensors, electrochemistry, and diagnostic technologies for pathogens like SARS-CoV-2 and HPV. She has published in leading journals such as Nature Communications and secured multiple national research grants for developing point-of-care testing systems using electrochemical DNA sensors and nanomaterials.

Analytical Chemistry (AC-I-052)

Power of analytical chemistry to solve the environmental and health problems

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Analytical chemistry deals with structural and chemical composition of matters by the help of qualitative and quantitative information. It helps to solve current problems such as microplastics, persistent organic pollutants, drug analysis, cancer diagnosis, coronavirus disease 2019 (COVID-19). Water pollution is another problem due to its potential risks for public health. These kinds of environmental and health problems can be eliminated or suppressed by analytical methods that give information about the presence and concentration of analytes. There are several analytical methods to determine organic, inorganic and biological compounds. Liquid (LC) and gas chromatography (GC) have been used to separate analytes found in complex sample matrices. Flame atomic absorption spectrometry (FAAS) is one of the most commonly used methods for the determination of metals. On the other hand, analytical instruments cannot handle matrix interferents or sensitivity problems. For this reason, sample pretreatment methods are necessary before analytical measurements. These methods can purify, concentrate and extract the analyte from complex sample matrices. Chloroquine, hydroxychloroquine, antidepressant drugs, endocrine disruptive compounds were extracted by liquid or solid phase extraction/microextraction methods prior to LC or GC systems. Heavy metals such as cadmium, copper, cobalt and nickel were determined by FAAS method after liquid or solid based phase extraction/microextraction methods. In addition, removal of organic and inorganic species was also performed using several adsorbents. Heavy metals, drugs, pesticides were treated with several nano-adsorbents for their removal from water matrices. Hence, trace determination of organic and inorganic analytes guides researchers to produce reasonable solutions for environmental and health problems.

Keywords: spectroscopy; chromatography; extraction methods; removal

Sezgin Bakirdere is a Full Professor of Chemistry at Yildiz Technical University. He earned his Ph.D. from Middle East Technical University in 2009. His research focuses on metal speciation, microextraction, hydride generation, food analysis, wastewater treatment, and chromatography. He has published over 370 papers, delivered more than 300 conference presentations, and authored books with CRC Press and Elsevier. A Full Member of the Turkish Academy of Science and a Fellow of the Royal Society of Chemistry, he also serves as an Executive Board member and Secretary General of the Turkish Chemical Society.

Analytical Chemistry (AC-I-053)

The convergence of electrochemistry and advanced materials: Paving the way for the next-generation analytical chemistry and miniaturized sustainable devices

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This presentation explores the intersection of electrochemistry, analytical chemistry, and advanced materials, demonstrating how their integration drives the development of next-generation analytical technologies and energy-autonomous systems. We highlight two key areas: (1) miniaturized electrochemical sensors and (2) enzymatic biofuel cells and self-powered biosensing platforms. Our work in sensor miniaturization includes wearable, implantable, ingestible, and portable devices for real-time monitoring in biomedical diagnostics, environmental surveillance, and food safety. Examples include printed bandage-based sensors with integrated pH correction for wound infection monitoring, flexible porous nanocomposite electrodes with tunable electrochemical properties, and diaper-embedded sensing arrays for noninvasive detection of ions and drugs. In parallel, we advance enzymatic biofuel cells by coupling bioelectrocatalytic systems with functional nanomaterials to enable efficient energy harvesting and self-powered biosensing. These innovations support the creation of sustainable and on-demand analytical tools that extend sensing capabilities beyond traditional laboratory settings. The discussion will also highlight how advanced materials are transforming electrochemical sensors and bioelectronics, contributing to the development of highly efficient, multifunctional devices. By showcasing recent breakthroughs, this presentation emphasizes the transformative potential of these interdisciplinary advancements for both fundamental chemical research and a broad range of real-world applications in healthcare, environmental monitoring, and sustainable technologies.

Keywords: electrochemical sensors; biofuel cells; wearable and implantable devices; advanced nanomaterials; self-powered biosensing

Itthipon Jeerapan is an Assistant Professor in the Division of Physical Science at Prince of Songkla University, Thailand. He earned his Ph.D. in Nano Engineering from the University of California San Diego. His research centers on electrochemistry, bioelectronics, wearable sensors, and advanced materials for medical, environmental, and energy applications. He serves as Associate Editor for ECS Sensors Plus and has received several prestigious awards, including the 2025 FACS Distinguished Young Chemist Award and the Thailand Young Scientist Award 2024. He has published over 70 papers with more than 5,450 citations.

Chemistry for Energy and Environment (CE-I-005)

Photoreforming of lignocellulose over single-atom Fe dispersed polymeric carbon nitride homojunctions

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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-N_4 sites. In addition, the Fe-N_4 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 presents universal applicability for photoreforming of various types of lignocellulosic biomass. [*ACS. Catal.* **2024**, *14*, 17321]

Keywords: photocatalysis; lignocellulose biomass; solar fuels; carbon nitride; single-atom catalyst

Can Xue received his Ph.D. in chemistry from Northwestern University in 2007. He is currently a tenured Associate Professor at the School of Materials Science & Engineering, Nanyang Technological University, Singapore. His research interests include developing new materials for solar energy applications such as light-driven solar-driven water splitting and CO2 reduction.

Chemistry for Energy and Environment (CE-I-007)

Organometallic materials and their applications in solar energy conversion

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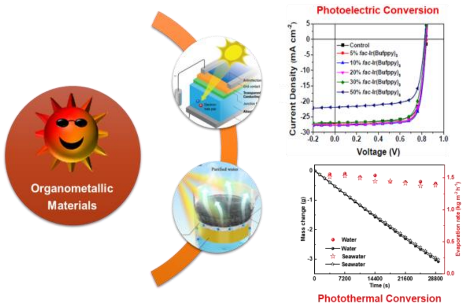
Solar energy technologies have gained significant global attention as crucial facilitators for the green and sustainable development of human society and the economy. Organic materials hold great potential in solar energy conversion due to their advantages, such as diverse molecular modification, pollution-free nature, low cost, solution processing, and flexible device fabrication. Our research focuses on developing novel organometallic polymers and investigating their performance in solar cells and solar evaporators. The iridium-based complexes with high singlet-to-triplet conversions would be explored to improve the exciton lifetime and diffusion length, while also optimizing the active layer morphology to enhance the efficiency of organic solar cells. Using this strategy, we have successfully improved the power conversion efficiency up to 18.45% and 18.54% for polymer solar cells with pseudo-planar heterojunction (PPHJ) and bulk heterojunction (BHJ) architectures, respectively. [*Chem. Eng. J.* **2025**, *507*, 160359; *Sci. Bull.* **2024**, *69*, 2862–2869; *Adv. Funct. Mater.* **2024**, *34*, 2411058; *Nano Energy* **2024**, *130*, 110174; *ACS Mater. Lett.* **2024**, *6*, 2964–2973; *Chem. Eng. J.* **2022**, 430, 132832] Additionally, a new strategy is proposed that integrates multiple charge transfer mechanisms, including metal-to-ligand, ligand-to-metal, ligand-to-ligand, and intermolecular charge transfers, into an organometallic polymer. We developed a new organometallic polymer, PffBTPt, which exhibits good photothermal performance due to its nearly full-solar-spectrum absorption property. [*J. Mater. Chem. A* **2024**, *12*, 9055–9065] The resulting solar evaporator exhibits a water evaporation efficiency of 85.6% and an evaporation rate of 1.57 kg m^{-2} h^{-1} under 1 sun, as well as achieves a 3-5 order of magnitude reduction in the concentrations of Ca^{2+}, K^+, Mg^{2+}, and Na^+ after desalination of seawater. This approach aims to design highly efficient photothermal materials for solar evaporation applications. The development of novel organometallic materials opens a meaningful pathway from molecular design to improving the solar energy conversion efficiency of both photo-to-electric and photo-to-thermal processes.

Keywords: organometallic polymer; organic solar cells; solar evaporator; photo-to-electric conversion; photo-to-thermal conversion



Miao Zhang received her Ph.D. from Beijing Jiaotong University (College of Science) in 2019. She is currently Research Assistant Professor at The Hong Kong Polytechnic University. Her research focuses on developing novel metal complexes for solar energy conversion, singlet and triplet exciton dynamic mechanisms, and organic memristor materials and devices.

Chemistry for Energy and Environment (CE-I-019)

Activation and deactivation of Fe-Al composite materials for production of turquoise hydrogen and nanostructure carbon

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Hydrogen is the leading candidate for accelerating the energy transition from fossil fuels to decarbonized, renewable energy systems. With the aim of producing turquoise hydrogen and solid fibrous carbon by methane cracking, to minimize the processing steps of carbon capture and storage technology, we synthesized mixed iron-oxide/alumina catalysts with Fe/Al molar ratio of 4-56, denoted as the 4-80FeAl samples, using the sol–gel method. Most of these catalysts, particularly the FeAl-4 catalyst with a Fe/Al mol ratio of 40, were highly active in methane cracking, thereby producing high quantities of hydrogen (mmol·g_{cat}^{-1}) and fibrous carbon (mmol g_{cat}^{-1}) at temperatures ≤750 °C for 6 h. *Ex situ* characterization, in situ TEM, and simulations revealed the mechanism governing the Fe/Al-catalyzed methane cracking. Although catalyst deactivation occurred via the reduction of the spinel alumina species with methane, it was significantly inhibited under mixed H_2–CH_4 flow, which enhanced stably secure the Fe–FeC^3 active species onto the spinel species. Our findings can benefit real-world circulation-system-based methane cracking processes.

Keywords: methane cracking; iron catalyst; reaction mechanism; hydrogen/methane co-feeding; lifetime enhancement

Shih-Yuan Chen received a Ph.D. (Chemistry) from National Taiwan University in 2008. He is currently a Senior Researcher at the National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan. His research topics focus on biofuels, ammonia, methane, and CO_2 conversion.

Surface and interfacial dynamics in energy materials

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The key to achieving net-zero CO_2 emissions by 2050 lies in our ability to convert renewable energy into storable fuels, with hydrogen playing a crucial role in connecting renewable energy sources to end-users. However, the challenge of producing hydrogen cost-effectively and on a large scale is complex. This challenge demands a thorough understanding of electrocatalysis to develop efficient catalysts. Designing stable and effective electrocatalysts for the challenging oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in water electrolysis is difficult, and we still lack a fundamental grasp of the processes that govern catalyst transformation and their ultimate performance and stability. Only by combining operando spectroscopy with electrochemical measurements can we gain a deeper understanding of the various phenomena occurring during the OER and HER. Current research in electrocatalysis primarily examines changes on catalyst surfaces. To understand how solid-liquid interfaces influence electrochemical processes, it is crucial to study the surface chemistry at the electrode-electrolyte boundary. In this presentation, I will demonstrate how the NSRRC beamlines provide essential insights into this area. Our experimental results underscore the importance of in-situ X-ray characterization in revealing the true mechanisms behind catalytic reactions.

Keywords: catalyst; X-ray; hydrogen evolution; oxygen evolution; in situ

Yan-Gu Lin received a Ph.D. (Material Science and Engineering) from the National Chiao Tung University in 2010. He is currently a research scientist at the National Synchrotron Radiation Research Center (NSRRC) in Taiwan. His research interests include energy materials, photoelectrochemical hydrogen generation, heterogeneous catalysis, electrochemical capacitors, and fuel cells.

Chemistry for Energy and Environment (CE-I-021)

Alkaline earth oxide-modified palladium catalysts for the highly selective partial hydrogenation of BDF fuel

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Chung-Kai Chang,[5] Dun-Yen Kang,[5] Nuwong Chollacoop,[4] Apanee Luengnaruemitchai[1,*]
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Soybean oil-derived biodiesel (SO-BDF) exhibits undesirable fuel properties such as low oxidative stability and poor cold flow property due to its high amount of polyunsaturated fatty acid methyl esters (poly-FAME). Partial hydrogenation is one of the key process to enhance these properties. This study develops new types of Pd/SBA-15 catalysts by impregnating Pd nanoparticles onto mesoporous silica SBA-15, followed by modification with alkaline earth metal oxides (Ba, Ca, and Mg) at a 0.5 alkaline to Pd molar ratio. The catalytic performance was evaluated for the partial hydrogenation of SO-BDF under mild reaction conditions (80 °C, 5 bar of H_2, 150 mL min−1 H_2 flow and 1000 rpm stirring), aiming to selectively hydrogenate poly-FAMEs into cis-monounsaturated FAMEs (cis-mono-FAMEs), generating products with good oxidative stability and cold flow properties with minimal saturated FAME and trans-mono-FAME formation. Among the catalysts tested, Ba-modified Pd/SBA-15 shows excellent hydrogenation activity, achieving the highest *cis*-C18:1content (68%), presumably owing to strong Ba-Pd interactions that facilitate the desorption of hydrogenated molecules. The Ba-Pd/SBA-15, with a Pd size of 8.2–10.3 nm, shows promising results for improving SO-BDF quality with high oxidative stability (>120 h). This study provides valuable insights for the sustainable industrial growth in the BDF sector.

Keywords: partial hydrogenation; biodiesel; palladium catalysts; alkaline earth metals; promotion effect

Apanee Luengnaruemitchai received B.Sc. (Chemistry) from Prince of Songkla University, M.S. (Chemical Technology) and Ph.D. (Petrochemical Technology) from Chulalongkorn University, Thailand. She is currently a full professor at The Petroleum and Petrochemical College, Chulalongkorn University. Her research interests include hydrogen and fuel cells, petrochemical and environmental catalysis, and biofuels.

Food, Agriculture, and Cosmetics (FA-I-005)

A challenge in green-extraction product utilization of Thai herbs in cosmetic formulation

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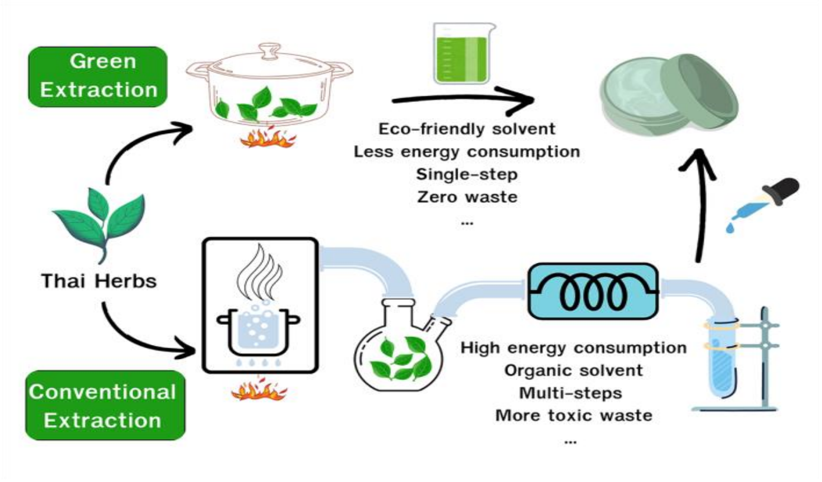
Many plants in Thai traditional medicine have potential as cosmetic ingredients. Typically, obtaining these ingredients involves multiple-step extraction with organic solvents, causing high energy consumption and waste. To improve the process, reducing steps and using eco-friendly solvents should be considered. Coincidentally, some traditional Thai herbal preparations align with modern green extraction principles, using renewable plant-based materials and fewer extraction steps at moderate temperatures with natural solvents. Nonetheless, fewer extraction steps can result in impurities and unpleasant textures, complicating modern cosmetic formulation and processing. This presentation will explore chemical concepts to resolve these issues, supported by real application case studies.

Keywords: green extraction; zero waste; Thai herbs; crude extract cosmetic formulation



Chak Sangma, PhD (born 23 July 1961), is an Assistant Professor at the Department of Chemistry, Faculty of Science, Kasetsart University. He earned his Ph.D. in Chemistry from the University of Leeds, UK, in 2000, and holds an MS and B.Sc. in Physical Chemistry from Mahidol University. His research areas including biosensors, virus identification, molecular modeling, and drug discovery from Thai traditional knowledge.

Food, Agriculture, and Cosmetics (FA-I-006)

Analytical approaches for GMO detection in food safety & compliance

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The growing presence of genetically modified organisms (GMOs) in global food production demands robust analytical methods to ensure regulatory compliance and food safety. Accurate GMO detection and quantification are essential for trade, labeling enforcement, and consumer transparency. This presentation highlights chemical and molecular analytical techniques, focusing on real time PCR (qPCR) as a widely used approach for GMO screening. In this study, 686 raw materials and food products (soy and maize) were analyzed between 2020 and 2024, sourced from various government and non-government agencies. Samples were screened for element-specific markers (CaMV 35S promoter, NOS terminator) and construct-specific markers (ctp2, cp4epsps) using qualitative PCR. Results showed 212 soy samples (53%) and 95 maize samples (33%) tested positive for GM elements/constructs, confirming the presence of at least one GM event. All soy and maize samples were confirmed using their respective taxon-specific genes (soy lectin and maize-specific gene). Given that soy and maize are primarily imported into Malaysia for food, feed, and processing, these findings underscore the need for a monitoring system to ensure effective GMO control. Beyond detection, challenges such as sample preparation, instrument calibration, method validation, and regulatory variations will be discussed. Additionally, the role of chemical-based approaches, including DNA extraction efficiency, in overall analytical performance will be explored. While PCR-based methods remain the gold standard for GMO detection, advancements in analytical chemistry could further enhance accuracy and reliability. This session will provide a practical perspective on GMO analysis, addressing laboratory challenges, regulatory considerations, and the need for harmonized testing methodologies to support food safety and international trade. Pragmatic, cost-effective, and time-saving approaches play a crucial role in ensuring the safety and sustainability of our food supply.

Keywords: GMO detection; qPCR analysis; food safety; regulatory compliance

Dr. Malarvili Ramalingam (born 1973) is the Director of the Biotechnology Division at the Department of Chemistry Malaysia. She holds a BSc (Hons) and MSc from the University of Malaya and a PhD in Environmental Science from Edith Cowan University, Australia. She specializes in analytical chemistry and environmental science, particularly in environmental analysis, emerging contaminants and food safety. She has received several awards, including the Excellent Service Award, the Director General's Award for identifying the geographical origin of Malaysian agro-products through isotopic and elemental fingerprinting, and the federal award Ahli Mangku Negara (A.M.N.) in 2021, conferred by the King.

Enhancing cosmetic efficacy: Stabilization and delivery of challenging active ingredients

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At the heart of skincare cosmetics lies their efficacy—determined by the potency of active ingredients and the effectiveness of their delivery to the skin. Achieving this efficacy is often hindered by the instability of certain compounds and the challenges of delivering them across the skin barrier. In this talk, we present two case studies that address these issues through formulation innovation. The first focuses on stabilizing and enhancing the dermal delivery of vitamins A and C, both of which are well-known for their rejuvenating properties but are chemically unstable and difficult to preserve in active form. The second case study highlights a novel technology for incorporating hydrophobic plant-derived actives—specifically α-mangostin and luteolin—into water-based formulations without the use of traditional surfactants. This approach not only maintains the bioactivity of these extracts but also improves their compatibility with sensitive skin. These examples showcase how the chemistry of self-assembly and bio-friendly polymerization can overcome long-standing limitations in cosmetic science and lead to more effective and skin-friendly skincare products.

Keywords :vitamin A; vitamin C; mangostin; luteolin

Born in 1968, after earning a BSc in Chemistry from Chulalongkorn University in 1986, Supason received her PhD in Chemistry from Miami University in 1992, in which she explored two different research areas, one in biochemistry focusing on the transportation of materials across cell membranes and the other in chemistry related to the chemical modification of the heparin drug and the structure-activity relationship study. Since then, she has been a faculty member at the Department of Chemistry, Chulalongkorn University. At Chula, she has authored more than eighty international publications in the fields of bioactive delivery, biomedical sciences, and medical devices.

Food, Agriculture, and Cosmetics (FA-I-013)

From DNA to health & beauty: Bioneer's 33 yrs history of R&D and business

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DNA synthesis and sequencing technologies have been the two wheels that have led the history of the genetic revolution. Dr. Park founded Bioneer Corporation in 1992 with two technologies: chemical DNA synthesis and polymerase-based DNA synthesis. He believed it was essential for Korea to develop gene technology and distribute it to Korean universities and research institutes. This would enable the effective utilization of gene technology to enhance the economy. As a result, he left the Korea Research Institute of Biotechnology and Bioscience (KRIBB) and founded Bioneer, which became the first biotech company in Korea. Bioneer has developed and produced five Nobel Prize-winning technologies for reading, writing, and regulating DNA, becoming the first in Korea to achieve this. He has invented new chemistries and instruments to address the practical limitations of applying these Nobel Prize technologies across various fields. Additionally, Bioneer has created and supplied numerous products that meet unmet needs while remaining affordable. For example, Dr. Park developed a high-sensitivity silver staining method that allows us to visualize small amounts of DNA in a sequencing gel without radioactive isotopes. This innovation has led to the world's first non-isotope Sanger sequencing method. To meet the high demand for oligonucleotides, he invented a matrix valve and developed the first 384-parallel oligo synthesizer. This innovation was instrumental in completing the fission yeast genome knock-out project, which aimed to discover the genes of cell division. By the application of RNA synthesis protocol, we successfully synthesized human gene siRNA and miRNA libraries consisting of over 100,000 oligonucleotides. The first libraries made in Asia play a significant role in the region's molecular cell biology research and drug development. Additionally, Bioneer created a mega-base oligo synthesizer to advance synthetic biology and established a biofoundry center. To prepare for the era of siRNA therapeutics, Bioneer also developed large-scale oligonucleotide synthesizers capable of producing tens to hundreds of grams of oligonucleotides. He also invented a faster, energy-efficient PCR instrument using copper nanowires and created real-time PCR instruments and automated nucleic acid purification instruments using magnetic nano-silica beads. Bioneer integrated its technologies into the molecular diagnostics system ExiStation. As a result, more than 90 countries worldwide have been able to diagnose COVID-19 using this equipment and reagents. Building on these advancements, he invented IRON-qPCR, a fully automated molecular diagnostic instrument that can detect 40 targets within 40 minutes. He invented a fully automated high-throughput molecular diagnostic instrument, ExiStation FA 96/384, which can conduct 94 tests in just 2 hours. The inventions will enhance precision medicine and improve pandemic preparedness. To overcome the hurdle of siRNA drugs, he invented a next-generation siRNA therapeutic platform called self-assembling siRNA (SAMiRNA), which enables the new drug development pipeline for fibrosis, cancer, and inflammatory diseases. Utilizing SMAiRNA's excellent safety profile and effective delivery to hair follicles, he created the world's first siRNA-based anti-hair loss cosmetic, CosmeRNA, a weekly hair tonic for both women and men. With its novel diagnostics and therapeutics platform, Bioneer is tackling significant challenges faced by humanity, such as pandemics, obesity, and hair loss. By combining fast molecular diagnostics with SAMiRNA-based antiviral drugs, Bioneer aims to create a world free from pandemics. Innovative basic science presents us with new opportunities to create new customer value. Let us appreciate cutting-edge basic science, create customer value through deep insights, and foster a safer, healthier, and happier life.

Keywords: DNA technology; oligonucleotide synthesis; siRNA therapeutics (samiRNA); molecular diagnostics

Dr. Han-Oh Park earned his bachelor's degree in chemistry from Seoul National University in 1984, followed by a master's degree in 1986 and a Ph.D. in 1992, both from KAIST. In 1992, he founded BIONEER Corporation, where he currently serves as Founder, CEO and Chairman. Dr. Park was the first in Korea to develop and commercialize Nobel Prize-winning technologies, including DNA synthesis, PCR, sequencing, siRNA, and miRNA. He has been honored with the Gold Tower Order of Industrial Service Merit for his contributions to the advancement of science and technology and the enhancement of Korea's bio-industry competitiveness.

Online methods in chemical education: The revolution is here

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The mode of teaching in Universities has not changed greatly for a century or more. The technology associated with the internet means that we can now make major changes as we move further further into the 21st Century. Then covid happened. As the pandemic spread in 2020, Universities scrambled to move to 100% online teaching with varying degrees of success. What can we learn from the experience of online teaching both in terms of being ready for the next pandemic and in terms of using the lessons learned in "normal" times.

The Division of Chemistry and Biological Chemistry at Nanyang Technological University (NTU) was established in 2005. Starting with a clean slate, an entire curriculum was developed including intensive synthetic chemistry labs. Extensive e-learning resources were put in place and have continued to be developed, and a strategy to ensure student involvement was designed.

Later, NTU launched a major initiative on "Technology Enabled Learning" (TEL). This enabled us to explore new different modes of teaching, using online methods to enhance instruction and free up time for active learning. Can we take advantage of technology to take a great leap forward in the quality of university education, or will it be much ado about nothing?

Keywords: online learning; active learning; e-learning; technology

Roderick Bates received his PhD at Imperial College, London. After a postdoctoral stint at Colorado State University with Professor L. S. Hegedus working on chromium carbenes, he moved to the University of North Texas as an Assistant Professor. After some years spent in Thailand at Chulalongkorn University and the Chulabhorn Research Institute and a short stay in the ill-fated Department of Chemistry at Exeter in England, he joined Nanyang Technological University as a pioneer member of the Division of Chemistry and Biological Chemistry. He is currently an Associate Professor and a Fellow of NTU's Teaching Excellence Academy.

Future in Chemical Education (FE-I-009)

Simple synthesis of gold nanoparticles (AuNPs) from gold leaf by electrolysis

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The combination of nanotechnology and chemical education provides new avenues and exciting activities for students. With the easily accessible resources and facile synthetic approach of electrolysis, we report herein a comprehensive hands-on experiment of synthesizing gold nanoparticles (AuNPs) from gold leaf in classrooms. The provided guidelines permit the teachers and students to perform laboratory activities for the synthesis of nanoparticles and learn the interactions between nanoparticles and light. AuNPs were synthesized in an aqueous solution containing sodium chloride (NaCl) as an electrolyte, glucose ($C_6H_{12}O_6$) as a reducing agent, and polyvinylpyrrolidone (PVP) as a stabilizing agent. During the COVID pandemic, this experiment was modified to allow students to perform it at home. The electrolytic solution was replaced by jelly without the addition of extra stabilizing agents or reducing agents. Moreover, the power supply was replaced by a 9-volt battery. The gold nanoparticles were successfully synthesized, but with a larger size. This experiment is valuable and effective, and the findings can be discussed in the context of learning about nanoparticle synthesis and their optical characteristics, which can be applied in high school and undergraduate students under supervision in classroom learning and remote education.

Keywords: gold leaf; gold nanoparticles; electrolysis; STEM education

Ekasith Somsook (b. 1972) received his Ph.D. in Chemistry from the University of Wisconsin-Madison. He is currently an Associate Professor at the Department of Chemistry, Faculty of Science, Mahidol University. His research focuses on catalysis for sustainability, particularly nanocatalysis, plastic recycling, and biorefinery.

Future in Chemical Education (FE-I-010)

Integrating chemistry education with sustainable development goals: a Bio-Circular-Green economy approach

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This presentation explores the integration of chemistry education with the Sustainable Development Goals (SDGs) through the Bio-Circular-Green (BCG) Economy Model. Using qualitative research methodologies, the study examines how STEM education approaches can be strengthened by embedding sustainability principles within chemistry curricula. The research investigates effective strategies for fostering innovative citizenship competencies among both teachers and students through hands-on, context-based learning activities. Findings reveal that successful chemistry education for sustainability requires contextualized instruction linked to real-world community challenges. Educators and students must be trained to identify environmental issues, apply analytical methods appropriately, and propose solutions aligned with BCG Economy principles. The presentation also offers practical frameworks for teacher professional development, emphasizing problem-solving strategies, green chemistry innovations, and assessment techniques adaptable across educational levels. Participants in these programs demonstrated enhanced scientific literacy, interdisciplinary thinking, ethical decision-making skills, and an increased ability to design sustainable innovations that connect chemistry concepts to community well-being. The presentation concludes with recommendations for chemistry educators aiming to integrate SDGs into their practice, thereby cultivating the next generation of sustainability-driven citizens.

Keywords: sustainable chemistry education; Bio-Circular-Green economy; STEM integration; citizenship competency; teacher professional development

Chatree Faikhamta (b. 1979) is an Associate Professor of Science Education and Associate Dean for Research and International Relations at the Faculty of Education, Kasetsart University. He holds a Ph.D. in Science Education from Kasetsart University. His research focuses on chemistry education, STEM integration, and pedagogical content knowledge (PCK), with an emphasis on teacher professional development. He leads nationally funded projects and has established research collaborations with partners in Canada, Japan, Korea, and Southeast Asia. He is currently co-developing the MII-STEM curriculum, emphasizing modeling-based instruction to strengthen chemistry and STEM teacher education.

Future in Chemical Education (FE-I-011)

Development of Chemistry Education Research (CER) as a field of inquiry and current status of CER in the world

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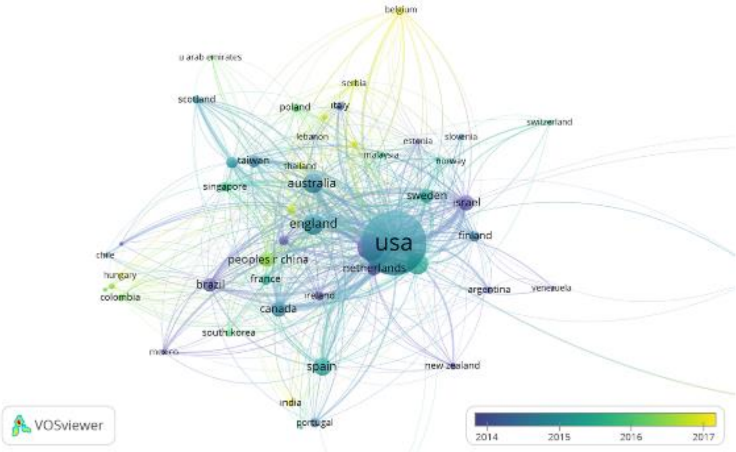
Chemistry education research (CER) could be considered as the inquiry aiming to improve the teaching and learning of chemistry. The wider scope of CER covers areas of research such matters as the chemistry curriculum; how learning of chemistry is assessed; the discipline specific aspects of how teachers are prepared for and developed in their work; the design of teaching resources that represent chemical knowledge in ways informed by knowledge of human learning processes or to support particular pedagogies [*Disc. Interdisc. Sci. Educ. Res*. **2019**, *1*, 1–8]. It is important to reveal the trends in the literature in order to develop solutions to meet these needs in chemistry education. With the determination of trends, current developments in chemistry education will be revealed and it will contribute to the planning of future research. This talk will focus on development of CER as a research field and continue with an analysis focusing on bibliometric data to show how CER is developed and what is the current status of the research output around the world. The findings will be presented in a comparative way to show the contribution of the different countries to CER.

Keywords: chemistry education research; development; history



Mustafa Sözbilir was born in 1973. He received his undergraduate and MSc degrees from Atatürk University/Türkiye in chemistry education and PhD in Educational Studies with a science education focus from the University of York/UK, in 2001. He is currently a full professor in chemistry education at the Department of Mathematics and Science Education at Atatürk University, Türkiye. His research interests include science/chemistry teacher training, students' learning in science/chemistry, undergraduates' understandings of chemical ideas in thermodynamics, trends in science/chemistry education research, and teaching science/chemistry to visually impaired students.

Future in Chemical Education (FE-I-012)

Integrating research into teaching and vice versa

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For many years, a key question in the chemical education research community is what evidence do we have about how to help students develop a deep and robust understanding of chemistry? A pre-requisite to addressing this question is that the instructor imparting the knowledge should hold a deep and robust understanding of chemistry, or at the very least, be aware of what they do not know.

In this talk, I will argue that this is quite often not the case by presenting two case studies from the teaching of (1) first year acid-base chemistry and (2) NMR analysis of the enolisation of β-diketones in a popular physical chemistry laboratory exercise. The talk will examine two common student questions – “when do mathematical strategies for approximating pH of weak acids break down?” and “why is enol the major isomer of β-diketones but not β-ketoesters?”.

The absence of readily available answers to these seemingly rudimentary questions in the literature has prompted the authors to conduct their own research to develop robust answers. This talk will present some of the findings in hope that it will equip the instructor with the deeper and robust understanding that will help enhance students’ understanding of fundamental chemistry.

Keywords: acid-base chemistry; enolisation; computational chemistry; pedagogical content knowledge

*Junming Ho is a research and teaching Associate Professor in the School of Chemistry at the University of New South Wales. He obtained his PhD from the Australian National University and has held research appointments at Yale and A*STAR. He is currently an Australian Research Council Future Fellow and was a recipient of the 2023 UNSW Award for Outstanding Contributions to Student Learning.*

Phosphorescent metal complexes for optoelectronic applications

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Phosphorescent metal complexes are attractive candidates for applications including organic light-emitting diodes (OLEDs), bioimaging, anti-counterfeiting, chemosensing, etc. In this talk, the recent advances on phosphorescent metal complexes of iridium(III) and platinum(II) will be discussed from the point of view of their structure–property relationships and the uses of these metallophosphors in high-performance OLEDs and organic solar cells will be described. Besides, new and efficient strategies to develop phosphorescent near-infrared emitters and soft salt complexes will also be presented and their optoelectronic applications will be presented.

Keywords: metal complexes; phosphorescence; color tuning; soft salts; optoelectronics

Wai-Yeung Wong obtained his B.Sc. and Ph.D. degrees from The University of Hong Kong. He completed his postdoctoral studies at Texas A&M University and University of Cambridge. Currently, he works at the Hong Kong Polytechnic University as Dean of Faculty of Science and Chair Professor of Chemical Technology. He was awarded the RSC Chemistry of the Transition Metals Award, FACS Distinguished Young Chemist Award and China's State Natural Science Award, among others. He is a Fellow of RSC and a Foreign Member of European Academy of Sciences. His research focuses on organometallic and materials chemistry, especially aiming at developing multifunctional optoelectronic materials.

Inorganic Chemistry (IC-I-023)

Symmetry-breaking and polymorphism in iron(III) spin crossover complexes

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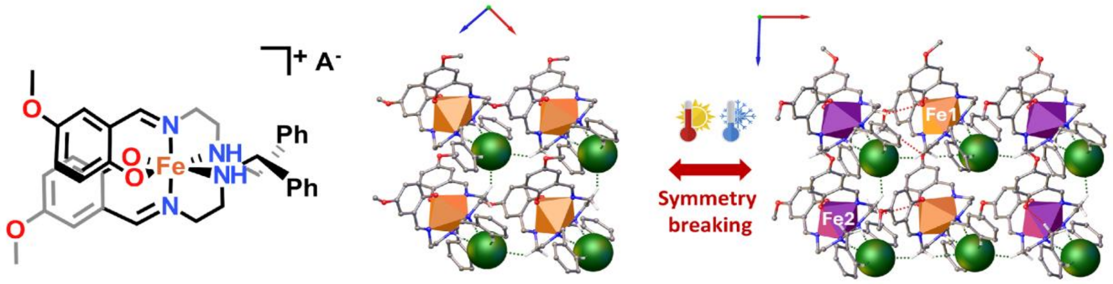
Spin crossover complexes exhibit a transition between a high spin (HS) and a low spin (LS) state stimulated by temperature, pressure, and light irradiation with potential for high-density data storage and sensors. In this talk the effect of different anions on spin crossover behaviour is discussed, including the decoupling of symmetry-breaking from spin crossover and polymorphism in some of these iron(III) compounds. The impact of the anions on redox behaviour their potential for anionic sensing is also described.

Keywords: spin crossover; magnetism; iron(III) complexes; hysteresis; sensors



Associate Professor Dr David J. Harding was born in 1976 in the UK and graduated with a B.Sc. at the University of Edinburgh in 1997 and a Ph.D. from the University of Bristol in 2000. He currently works at Suranaree University of Technology where his research interests are in the discovery of materials with designed structural, optical and magnetic properties for molecular electronics. He is a fellow of the Royal Society of Chemistry, FRSC, and recipient of the Dalton Transactions: New talent Asia Award in 2014.

Inorganic Chemistry (IC-I-026)

Azo-coupling chemistry in a flow

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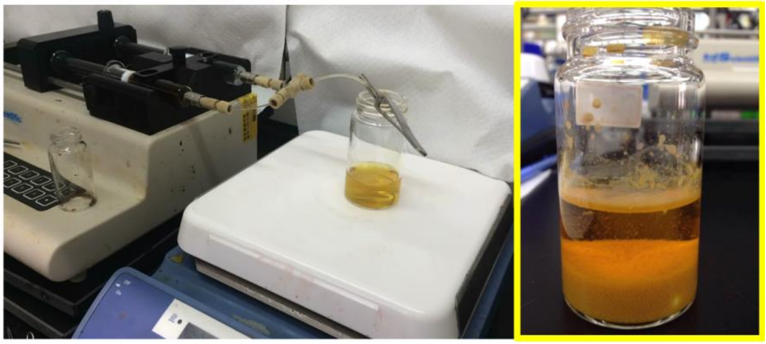
The presentation includes firstly a discussion on the difference of a batch reaction from a flow reaction. In a batch reaction, the reactants exhibit a broader range of thermal distribution allowing access to varying possible reaction pathways and hence varying possible products. In a microfluidic setup, special notes are taken on tubing inner diameter (10–500 μm) and surface area (1–5 × 10^4 m^2/m^3). The thermal energy distribution is much narrower in a flow reaction. Secondly the presentaton gives examples specifically on the azo-coupling reaction, optimizing in general the flow rate, the reactant molar ratio, the length of tubing for the reaction from start to stop, etc. The azo-dyes are easily produced, purified, and characterized. The presentation further extends to metal-azo complexes, in which an azo-coupling produces in a flow system the acid dyes that are Cr- or Fe-coordinated to exhibit versatile solvent exchange behavior.

Keywords: azo-coupling reaction; flow reaction; metal-azo complex



Ling-Kang LIU is emeritus research fellow in the Institute of Chemistry at Academia Sinica. He obtained his B. S. in 1972 from National Taiwan University and obtained his Ph. D. in 1978 from University of Texas at Austin. He started his career at Academia Sinica since 1979 and later became also adjunct professor in National Taiwan University. His research interests were in inorganic chemistry and in ionic liquids. After his retirement, he had served in 2019-2023 as the Secretary General of FACS. Ling-Kang LIU receives a citation in 2025 from FACS.

Inorganic Chemistry (IC-I-027)

Sustainable synthesis of heteroarenes via heterogeneous (photo)catalyzed C–H bond functionalization

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Since heterocyclic aromatic compounds form the structural core of many pharmaceuticals and biologically active molecules, their efficient synthesis is a major focus in synthetic organic chemistry [*Eur. J. Med. Chem.* **2020**, *208*, 112783]. Traditionally, carbon–carbon (C–C) cross-coupling reactions such as Suzuki–Miyaura, Sonogashira, Stille, and Heck have been widely employed for this purpose. However, these methods often require substrate pre-functionalization, high reaction temperatures, and the use of noble metal catalysts—factors that limit their sustainability and scalability. In this context, direct carbon–hydrogen (C–H) bond functionalization has emerged as a powerful and environmentally friendly alternative, offering atom- and step-economical access to C–C bonds without pre-activation of substrates [*Chem. Soc. Rev.* **2011**, *40*, 1855–1856]. While homogeneous metal catalysts have shown high activity in C–H functionalization, issues related to recovery and recyclability hinder their practical application. To address these challenges, heterogeneous catalytic systems have been explored, offering advantages in catalyst reuse and operational simplicity. Yet, high temperatures and extended reaction times often remain necessary. Recently, photoredox-catalyzed C–H functionalization has attracted growing attention as a sustainable route, using visible light to promote reactivity under milder conditions [*J. Am. Chem. Soc.* **2012**, *134*, 2958–2961].

In this presentation, I will highlight our recent studies in the development of heterogeneous (photo)catalysts for the direct C–H arylation of (hetero)arenes. Specifically, I will discuss the catalytic performance of reduced graphene oxide-supported Ni/Pd core–shell and NiPd alloy nanoparticles. Additionally, I will present our work on metal-free, two-dimensional (2D) semiconductor photocatalysts—including black phosphorus, nitrogen-vacancy graphitic carbon nitride, bismuthene, and heterojunction structures—for visible-light-induced C–H arylation of (hetero)arenes.

Keywords: C–H bond functionalization; heterogeneous catalysis; photoredox catalysis; heteroarenes

Dr. Önder Metin earned his PhD in Chemistry from Middle East Technical University in 2010. He was a visiting scholar at Brown University (USA) in 2009 and Darmstadt Technical University (Germany) in 2010, and a postdoctoral researcher at Brown University from 2012 to 2013. He has received several prestigious awards, including TUBITAK's Research Encouragement Award (2017) and the Turkish Academy of Sciences' Young Scientists Award (2014). His research focuses on transition metal nanoparticles, 2D materials, and nanocomposites for applications in catalysis, hydrogen storage, and sustainable chemistry. Dr. Metin has published over 160 papers, garnering more than 10,000 citations and an h-index of 52.

Materials Science and Nanotechnology (MN-I-002)

Hexagonal boron nitrides: Their applications from nanomedicine to nanophotonics

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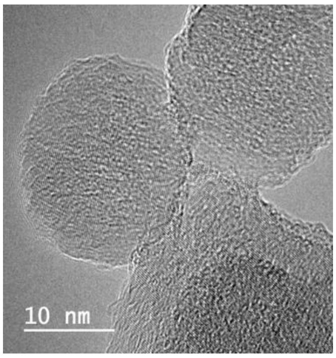
Hexagonal boron nitrides (hBNs) are 2D nanomaterials with unique physicochemical properties. They are formed by the covalent bonding of boron (B) and nitrogen (N) atoms in a hexagonal pattern similar to graphene. Thus, their properties are often compared but they have rather different properties due to the difference in the electronegativity of the B and N atoms compared to the C-C bond in graphene, where the electron cloud in the σ bond is more localized on N atom. The bond π consists of an empty p orbital of B and the full orbital p of N. In this way, the electrons of N are less delocalized. Therefore, the bond is more ionic and the symmetry of the electronic state is broken. Due to this electronic structure, the band gap is rather wide (~5.9 eV), and as a result, they lose their electrical conductivity. However, this electronic structure brings other novel photonic properties including single photon emission. The hBNs have also attracted the attention of biomedical researchers in recent years due to their biocompatibility, low toxicity, and potential use in neutron capture therapy, drug delivery, and cancer therapy through their degradation products. In this talk, I will present our effort to utilize these unique nanomaterials as nanocarriers, cancer therapeutics, and single photon emitters.

Keywords: hexagonal boron nitrides; drug delivery; nanophotonics; quantum emitters



Mustafa Culha obtained his Ph.D. at the University of Tennessee-Knoxville. His research interests include analytical, bioanalytical chemistry, and nanobiotechnology. He is a Fellow of the Society for Applied Spectroscopy and the president of The Federation of Asian Chemical Societies (FACS) from 2023-2025. He serves as Associate Editor for Frontiers Nanobiotechnology, and on the editorial board of Applied Spectroscopy, Biology, Applied Sciences, and Journal of Molecular Structure.

Materials Science and Nanotechnology (MN-I-016)

A simple, inexpensive and general photoluminescent sensor platform for multiple analytes

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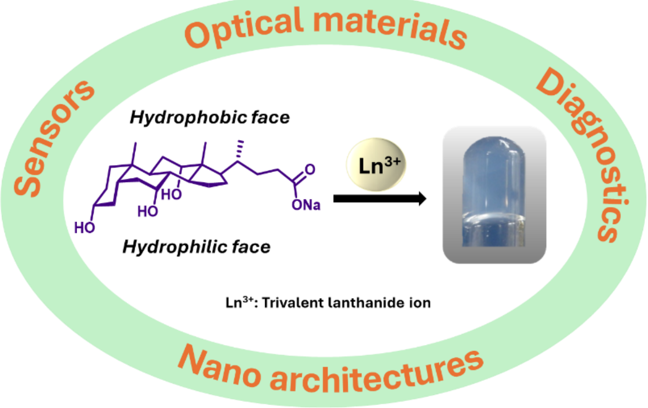
Almost 15 years ago, we discovered a facile method to enhance the luminescence from lanthanides through the self-assembly of multiple components in a metallohydrogel. Using this strategy, we have developed a masked sensitizer ("*pro*-sensitizer") based protocol for sensing enzymes and a few small molecules. We have also found that some natural products and clinically used drugs can sensitize lanthanides. The gel-based platform, therefore, provides opportunities to detect and quantify such species as well. This talk will highlight the progress we have made in this area focusing on the work done during the past 2–3 years.

Keywords: photoluminescence; lanthanides; hydrogels; enzymes



Uday Maitra is an Honorary Professor at the Indian Institute of Science (IISc) Bangalore. He received his Ph.D. from Columbia University and completed postdoctoral research at the University of California, Berkeley. His research focuses on hydrogels, hybrid materials, and low-cost, paper-based photoluminescent sensors for biological analytes. A dedicated advocate for chemistry outreach, he is a Fellow of both the Indian Academy of Sciences and the Indian National Science Academy and currently serves as President of the Chemical Research Society of India (CRSI).

Materials Science and Nanotechnology (MN-I-028)

Plasma bio-engineering: Advancing biomimetic devices, biofabrication, and nanomedicine

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The prevalence of implantable medical devices has witnessed a significant rise on a global scale, with an annual occurrence of hundreds of thousands of procedures. However, a substantial portion of these procedures experience complications, frequently associated with infections or insufficient integration with the host tissues. Implementing strategic surface functionalization with bio-instructive properties offers a viable approach to regulate biological reactions and direct the differentiation of stem cells through surface-attached biomolecules and hydrogels. Here, we showcase the remarkable capabilities of plasma bio-engineering techniques in crafting such instructive interfaces on a diverse array of materials. These materials span a spectrum of chemistries and geometries, including titanium, stainless steel, bioceramics, and polymers such as ePTFE and silk. Our findings provide evidence on the covalent immobilization of multifunctional protein layers, peptide molecules with preferred orientation, hydrogel coatings, and even silver nanoparticles on the plasma-engineered surfaces. These modifications lead to improved cellular responses and bolstered antimicrobial properties, validated for a broad range of biomedical engineering applications, from surface engineering of bone implantable devices to creating constructs for cartilage tissue regeneration. The plasma bio-engineering approach holds significant promise for developing the next generation of bioactive materials and interfaces, not only for biomedical implant applications but also for broader medical advancements.

Keywords: plasma processes; biomaterials; biointerfaces; tissue engineering; hydrogels

Behnam Akhavan is an Associate Professor of Biomedical Engineering at the University of Newcastle, Australia, and an ARC DECRA Fellow. He leads the Plasma Bio-engineering Laboratory at the School of Engineering and Hunter Medical Research Institute. After earning his Ph.D. in Advanced Manufacturing from the University of South Australia in 2015, he held research positions at the Max Planck Institute, Fraunhofer Institute, and the University of Sydney. His research focuses on plasma surface bioengineering, with over 80 publications, and he has been named one of Australia's Most Innovative Engineers by Engineers Australia.

Materials Science and Nanotechnology (MN-I-031)

Optimization of the electrophoretic deposition process of recycled γ-alumina coating on titanium for biomedical applications

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Kusuma P. Suwondo,[2] Juhrotul Uyun,[4] Muhammad P. Kamil,[2] Muhammad Kozin,[2]
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The coating of gamma alumina (γ-Al_2O_3) from recycled materials has been successfully applied to Cp-Ti using the EPD (Electrophoretic Deposition) method. This study aims to analyze the influence of EPD parameters on the resulting recycled γ-Al_2O_3 coating. The γ-Al_2O_3 was synthesized from cans wastes using the sol-gel method. The coating of γ-Al_2O_3 on Cp-Ti was carried out using the Taguchi experimental design (DoE) approach to optimize EPD parameters such as pH, concentration, and voltage. Characterization of γ-Al_2O_3 was performed using XRD, FTIR, Particle Size Analyzer (PSA), BET, and zeta potential for the γ-Al_2O_3 suspension. Furthermore, the γ-Al_2O_3 coating was characterized using 3D OM, XRD, and SEM-EDS. Corrosion testing was conducted using simulated body fluid (SBF). The recycled alumina showed XRD diffraction peaks at 2θ angles of 32.06°, 37.84°, 45.98°, and 67.17°, indicating the γ-phase. FT-IR analysis revealed absorption bands at 513 cm^{-1} for octahedral Al-O bending vibrations and 820 cm^{-1} for tetrahedral Al-O bending vibrations. The γ-Al_2O_3 had a particle size distribution of 314 nm, with a pore size of 2.45 nm. The results showed that EPD parameters at pH 2, a concentration of 5 g/L, and a voltage of 30 V yielded high deposition efficiency and homogeneity. Based on the delta S/N ratio values of 16.66 and 3.97, pH was the most influential parameter on the coating results, including deposition efficiency and homogeneity. The order of parameters affecting the coating results was pH > concentration > voltage. A pH of 2 showed a zeta potential of +9.56 mV with a mobility of 0.2697 $cm^2/V\cdot s$. The γ-Al_2O_3 coating exhibited roughness in the range of 1.58–2.38 µm. The optimal parameters produced a coating with a roughness of 1.91 µm, which falls within the ideal roughness range for implants. The alumina coating also maintained its phase as γ-Al_2O_3. The corrosion potential of γ-Al_2O_3-coated Cp-Ti showed an *Ecorr* value of 232.17 mV, higher than that of uncoated Cp-Ti (*Ecorr* -845.71 mV). Additionally, γ-Al_2O_3-coated Cp-Ti had an *Icorr* value of 9.10×10^{-7} A/cm^2 and a polarization resistance (*Rp*) of 3.82×10^{4} $\Omega\cdot cm^2$. These results indicate that the recycled γ-Al_2O_3 coating on Cp-Ti significantly enhances corrosion resistance compared to uncoated Cp-Ti.

Keywords: Cp-Ti; gamma alumina; electrophoretic deposition; implant

Fitri Khoerunnisa is a Professor of Chemistry at Indonesia University of Education. She earned her Ph.D. in Chemistry from Chiba University, Japan, in 2011 and completed postdoctoral research at Shinshu University from 2011 to 2016. Her research focuses on carbon nanomaterials and nanocomposites. She holds patents in Japan and Indonesia and has received honors including the Loreal-UNESCO For Women in Science Fellowship (2016) and National Academic Leader in Science (2018).

Materials Science and Nanotechnology (MN-I-048)

The outstanding performance of mesoporous I-doped-G-C_3N_4 photocatalyst for antibiotic removal under visible-light irradiation

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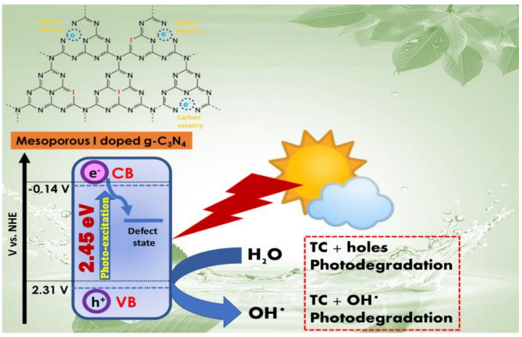
The development of graphitic carbon nitride (g-C_3N_4, GCN) as a photocatalyst has garnered significant attention for the removal of antibiotic pollutants from wastewater. However, its practical application is hindered by rapid electron–hole recombination, limited surface area, and poor visible light absorption. In this study, a series of mesoporous iodine-doped GCN (I-GCN) photocatalysts were synthesized, with GCN-I0.50 (0.50 g of I dopant) demonstrating optimal performance. Under visible light irradiation ($\lambda > 420$ nm), GCN-I0.50 achieved 99.8% degradation of tetracycline (TC) within 150 minutes, exhibiting a 2.64-fold enhancement in photodegradation rate compared to pristine GCN. The incorporation of iodine and the formation of carbon vacancies facilitated electronic reconstruction, enhancing charge separation and creating additional active sites. The mesoporous architecture and increased surface area (63.76 m^2/g) further contributed to efficient pollutant adsorption and degradation. Additionally, structural distortion induced by iodine doping enabled n–π^* transitions and reduced the band gap to 2.45 eV, extending photoactivity into the visible range. The GCN-I0.50 photocatalyst exhibited remarkable photocatalytic efficiency and stability, highlighting its potential for wastewater treatment applications.

Keywords: iodine; graphitic carbon nitride; photocatalyst; tetracycline; mesoporous



Juan Joon Ching is a Professor of Chemistry at Universiti Malaya, specializing in nanomaterials for environmental and energy applications. With over 200 WoS-indexed publications and an h-index above 50, he has been named among Stanford's Top 2% Scientists (2020–2024). His honors include the IKM Gold Medal (2024) and National Young Scientist Award (2016). He is a Fellow of the Royal Society of Chemistry and holds leadership roles as President of Balai Ikhtisas Malaysia, NR/AM of IUPAC, and Founder of MYCN-IKM, actively advancing national and international scientific communities.

Materials Science and Nanotechnology (MN-I-051)

Impact of nanomaterials on membrane performance enhancement

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The global membrane separation technology market size was valued at USD 28.4 billion in 2023 and the worldwide membrane separation technology market size is expected to reach USD 90.6 billion by 2033. As global warming, environmental challenges, industrialization, and population growth intensify, ensuring a circular economy and sustainable development becomes increasingly critical. Membrane technology has emerged as a strategic tool to meet global resource demands due to its low energy consumption, modular flexibility, and adaptability to hybrid processes. Despite its widespread application in separation and purification processes, current polymeric membranes face significant challenges, including fouling, limited selectivity, non-uniform pore size distribution, and reduced performance under high temperatures or prolonged solvent exposure. These drawbacks necessitate innovative material integration and advanced membrane designs to enhance performance, mechanical durability, thermal and chemical resistance, and lifespan while maintaining high permeability and selectivity.

Recent advancements in nanotechnology and materials science have paved the way for next-generation membranes that address these limitations. The precise engineering of nanoscale pore channels and functionalities using 2D materials such as graphene, graphene oxide (GO), reduced graphene oxide (rGO), hexagonal boron nitride (hBN), carbon nanotubes (CNTs), and metal-organic frameworks (MOFs) has demonstrated remarkable potential. These materials enhance filtration efficiency, fouling resistance, and mechanical stability, while enabling tunable pore size and functionality for diverse water treatment applications, including desalination, dye removal, and pollutant degradation. Incorporating nanoparticles such as multi-layered CNTs and TiO_2 into membranes further improves filtration quality, fouling resistance, and photocatalytic activity. Strategies like metal doping and surface modifications enhance TiO_2's photocatalytic efficiency, particularly under visible light, while CNTs serve as robust support materials, improving both structural integrity and reactive properties. In addition, block copolymer (BCP) technology also enables the fabrication of nanoporous membranes with narrow pore size distributions, high porosity, and tailored chemical and mechanical properties, offering scalable and cost-effective solutions for advanced separations.

The synthesis, characterization, and application of these advanced materials to create mixed matrix membranes (MMMs) and thin-film composite nanomembranes (TFNMs) have been widely focused. By integrating multi-layered CNT-modified TiO_2 nanoparticles into polysulfone/polyamide composites, the resulting membranes exhibit high permeability, reduced fouling, and excellent mechanical stability, making them ideal for drinking and industrial water treatment. Furthermore, machine learning approaches are explored to optimize membrane design and performance, addressing challenges experimentally and computationally.

By integrating nanotechnology, polymer chemistry, and interdisciplinary collaboration, these innovations provide disruptive, environmentally stable materials for advanced separations. They contribute to sustainable water management, aligning with the principles of responsible chemical sciences and addressing global sustainability goals through cutting-edge research and development.

Keywords: nanocomposite membrane; nanomaterials; 2D materials; water treatment

Mustafa Ersoz is a Professor of Chemistry at Selcuk University, Turkey, specializing in physical chemistry, membrane technology, nanochemistry, and surface chemistry. He earned his Ph.D. from Glasgow University in 1994 and held fellowships and visiting positions in Germany and the UK. He has led major national and international projects, including several EU Framework and H2020 programs. A founding director of multiple research centers, he has received the Junior Scientists Award (1998) and Scientists Award, and currently serves as a full member and Council member of the Turkish Academy of Sciences (TUBA). He has published over 160 scholarly articles.

Materials Science and Nanotechnology (MN-I-052)

Tailoring morphology and electronic properties in nanostructured alloy-chalcogenides: A paradigm for sustainable photo-catalysis

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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 underscores their potential as model systems for sustainable catalysis research, paving the way for their application in future catalytic technologies.

Keywords: photocatalysis; chalcogenides; alloys; nanostructures; multifunctional

Kalyanjyoti Deori is an Assistant Professor of Chemistry at Dibrugarh University, India. He earned his M.Sc. and Ph.D. from the University of Delhi and previously taught at Kirori Mal College, University of Delhi. His research focuses on advanced functional nanomaterials for catalytic applications, including sustainable photocatalysis, electrocatalysis, and energy conversion. He has an extensive publication record, multiple patents, and has received several honors, including the University Teacher Award-2023. His work contributes to advancing sustainable chemistry and environmental technologies.

A game of terpenes: Structure, stereochemistry and biosynthesis of terpenoids from marine animals

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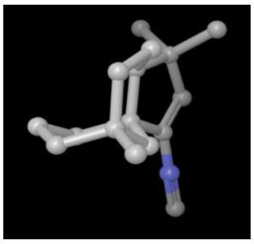
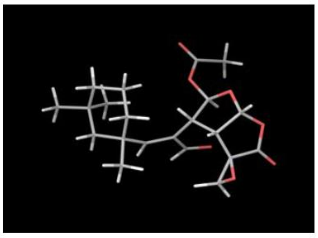
This talk will describe how an ecological study on chemical defense in nudibranchs led to the isolation and characterization of new terpene metabolites with extensively-rearranged carbon skeletons. Case studies that will be discussed include new isocyanoterpenes from phyllidid molluscs [*J. Nat. Prod.* **2015**, *78*, 1422–1427; *J. Org. Chem.* **2017**, *82*, 13313–13323] and epoxy-substituted norditerpenes from *Goniobranchus* spp. [*ACS Omega* **2017**, *2*, 2672–2677; *J. Nat. Prod.* **2020**, *83*, 714–719]. NOESY data run at 700 or 900 MHz, together with detailed conformational analyses informed by molecular modeling, DFT calculations, and in one example total synthesis in collaboration with a USA laboratory, enable assignment of individual configurations. The chemistry data are reviewed in an ecological and biosynthetic context.

Keywords: terpenes; NMR spectroscopy; nudibranchs; sponges; stereochemistry





Mary Garson is Professor Emerita at the University of Queensland in Brisbane. She completed her PhD at the University of Cambridge in 1977, and then held research or academic positions in Rome, Townsville, and Wollongong. She is a Fellow of the Australian Academy of Science and President-Elect of the International Union of Pure and Applied Chemistry. In 2019, she became a Member of the Order of Australia for her significant service to education.

Natural Products, Biological Chemistry and Chemical Biology (NB-I-039)

Elucidating the biosynthesis of menisporopsin A, a fungal macrocyclic polylactone

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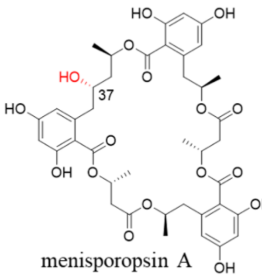
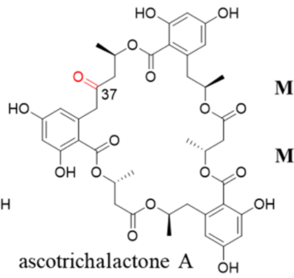
Menisporopsin A is a bioactive macrocyclic polylactone with potent antifungal activity, produced by *Menisporopsis theobromae* BCC 4162. Its biosynthetic pathway was previously proposed based on the ^{13}C labelling results and transcriptomic analysis during the production phase of menisporopsin A revealed two highly expressed polyketide synthase (PKS) genes, *men1* encoding reducing PKS and *men2* encoding non-reducing PKS, as likely candidates. Heterologous expression of these genes in *Aspergillus oryzae* NSAR1 was sufficient to produce ascotrichalactone A, a non-reduced C-37 analogue of menisporopsin A. Multiple esterifications and cyclolactonisation likely rely on Men2, which contains tandem acyl carrier protein (ACP_1-ACP_2) and thioesterase (TE) domains. Site-directed mutagenesis of the doublet ACP showed that ACP_2 alone is sufficient for constructing the aromatic subunits of menisporopsin A, whilst ACP_1 is capable of carrying products from multiple esterifications of the non-aromatic subunit, 3*R*-hydroxybutanoic acid. These findings provide deeper insight into macrocyclic polylactone biosynthesis and support future engineering of this class of bioactive compounds.

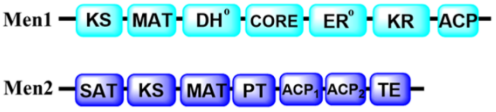
Keywords: menisporopsin A; biosynthesis; polyketide synthase; heterologous expression



menisporopsin A



ascotrichalactone A



Pakorn Wattana-Amorn

Education: Ph.D., University of Bristol (2007)
Current Position: Associate Professor, Department of Chemistry, Faculty of Science, Kasetsart University
Research interests: Heterologous expression of natural product genes, biosynthetic studies of natural products and biological NMR.

Natural Products, Biological Chemistry and Chemical Biology (NB-I-040)

Antiviral and virucidal natural products against SARS-CoV-2, influenza A virus (H1N1), HSV-2, and enterovirus 71

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The pandemic of SARS-CoV-2 (COVID-19) virus caused more than 7 million deaths worldwide (WHO report, March 2025), and it also had the largest impact on global economic and affected daily life of people. The COVID-19 pandemic, as well as a recent mysterious flu-like undiagnosed disease, known as a “Disease X”, in Democratic Republic of Congo, suggests that there is an urgent need to search for new antiviral and virucidal compounds. Moreover, viruses have more pandemic potential than other human pathogens. We started our work on antiviral compounds just before the COVID-19 pandemic, and we first submitted a manuscript in November 2021 on antiviral natural products, while many countries in the world went into lockdowns because of the COVID-19 problem. Because of the COVID-19 pandemic, we tried to search for new antiviral and virucidal compounds, and discovered many antiviral and virucidal natural products, e.g., limonene, a peptide, flavonoid glycosides, procyanidin condensed tannins of (–)-epicatechin, tiliacorinine, dioscorine, racemosol, terrain, polyhydroxylated fatty alcohols, an anisole derivative, 5,7,4’-trimethoxyflavone, and lotus alkaloids, neferine and nuciferine (and their salts). This lecture will highlight antiviral and virucidal agents against SARS-CoV-2 from Kratom, *Mitragyna speciosa* (procyanidin condensed tannins of (–)-epicatechin), *Nelumbo nucifera* (neferine, nuciferine and their salts), and a Thai ginseng, *Kaempferia parviflora* (5,7,4’-trimethoxyflavone).

Keywords: natural products; antiviral compounds; virucidal compounds; COVID-19; virus pandemic

Prasat Kittakoop was born in September, 1965, and received B.Sc. (1st Class Honors, Chemistry) from Chiang Mai University, Thailand, and Ph.D. (Biochemistry) from University of Wales, Swansea, UK. Currently, he is a Professor at Chulabhorn Graduate Institute (CGI). His research interests are chemistry of natural products, green chemistry, and medicinal chemistry. Since 2020, he has been recognized as the World Top 2% Scientists in Medicinal & Biomolecular Chemistry, based on the number of Scopus citations (h-index 47, 6,020 citations, retrieved on 9 April 2025). He is a regular reviewer of many journals.

Organic Synthesis and Medicinal Chemistry (OM-I-031)

One-pot synthesis of dibenzo[*b*,*f*]oxepines: Applications to the synthesis of anticancer pacharin, bauhiniastatin 4, bauhinoxepins C and D

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Phanida Thongaram, Panitan Kraikruan, Adisak Thanetchaiyakup, Wiradet Siri,
Asamaporn Tieojaroenkita, Nutthawat Chuanopparat, Paiboon Ngernmeesri*
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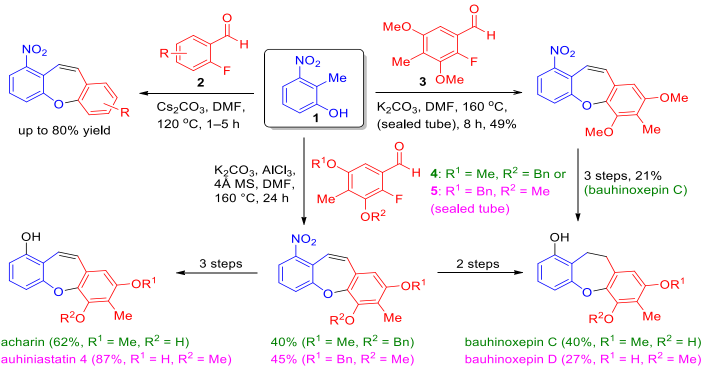
Pacharin, bauhiniastatin 4, and bauhinoxepins C and D are bioactive natural products featuring a dibenzo[*b*,*f*]oxepine core with significant anticancer activity. In this study, we report a novel and efficient one-pot synthesis of dibenzo[*b*,*f*]oxepine derivatives via a cascade process. The method involves an intermolecular nucleophilic aromatic substitution between 2-methyl-3-nitrophenol (**1**) and 2-fluorobenzaldehyde derivatives (**2**), followed by an intramolecular Knoevenagel condensation. Employing benzaldehyde **3**, prepared from 2-methylresorcinol, in this cascade reaction enabled the synthesis of bauhinoxepin C in 7 steps with an overall yield of 5.1%, featuring a final selective demethylation step. For the synthesis of the other natural products, selective benzylation and methylation strategies were applied to convert 4-methylresorcinol, obtained from 2-methylresorcinol, into benzaldehydes **4** and **5**, respectively. Pacharin and bauhiniastatin 4 were then synthesized from benzaldehyde **4** with overall yields of 5.4% and 8.3%, respectively (8 steps from 2-methylresorcinol), while bauhinoxepins C and D were obtained from benzaldehyde **5** with overall yields of 3.5% and 2.6%, respectively (7 steps from 2-methylresorcinol).

Keywords: natural product synthesis; one-pot synthesis; cascade reaction; dibenzo[*b*,*f*] oxepine; anticancer



Paiboon Ngernmeesri received his Ph.D. in chemistry from Pennsylvania State University in 2008. Subsequently, he began his academic career at the Department of Chemistry, Faculty of Science, Kasetsart University, where he currently holds the position of Associate Professor of Organic Chemistry. His research interests lie in the development of innovative synthetic methodologies and their application in the total synthesis of natural products.

Organic Synthesis and Medicinal Chemistry (OM-I-033)

Conformational constraint in organic & bioorganic chemistry

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Molecular shape recognition is a key for biological activity, which may derive from the stereochemistry of organic molecules. So that the stereochemical control is of apparent significance in the multi-step synthesis of natural products. This author uses *'conformational constraint'* as a concept controlling possible stereoisomers by the following factors: (1) rendering the molecular conformation and (2) enforcing direction of the reactants to approach each other. For the bond making/braking process, molecular orbital overlap is indispensable under limited orientation at the transition state. Important factors making the reactants in proper arrangements are (i) acyclic allyl strain (ii) stereoelectronic factor, and (iii) chelation control. Synthetic methodologies designed along this line are HeteroAtom Directed Conjugate Addition to make C-C bond either *syn* or *anti* diastereocontrol and further functional group transformation. Alpha selective C-glycosidation is another example with silyl-acetylene, which was used in various natural product synthesis. Cobalt-acetylene chemistry has been developed to assist ether-ring cyclization. After use, it also works for regiospecific hydro-silylation and ketone-synthesis, which are the other examples of *conformational constraint* by rendering the substrate-shape to result in the stereo-specific reactions. This principle has been established during the course of total synthesis of maytansine, okadaic acid, tautomycin, tetrodotoxin, ciguatoxin, and other complex natural products. Stereochemical process was even found in the biochemical events happening on protein surface, where it takes place even with non-stereogenic substrate. In our bioluminescence studies, a chromophore, dehydro-coelenterazine (having no chirality) involves significant stereochemical process by making 2 covalent bonds with 390-Cys of the photo-protein, symplectin, and molecular oxygen. In fact, one diastereoisomer emits strong light, but the other isomer not, and both of them end up with non-stereogenic products. We call this situation as *dynamic chirality* happening only with protein surface as significant stereochemical issue in bioorganic event.

Keywords: conformational constraint; dynamic chirality; stereoelectronic effect

B 1944, Nagoya Univ. PhD 1973, Postdoc Columbia U., Assoc. Prof. NU 1975-1991, Prof. NU 1991-2008, Prof. Emeritus NU 2008~present, Chair Prof. Nat. Tsing Hua U 2008-2014, Chair Prof. Nat. Sun Yat-Sen U 2014-1015, Vis. Prof. Chinese U Hong Kong 2015, Prof. Chulabhorn Res. Inst. 2015-2016, Vis. Prof. Toyama Pref. U 2017~. Purple Ribbon 2008, Princess Chulabhorn Gold Medal 2012, Order Sacret Treasure-Gold Rays 2018, JCS-ACS Nakanishi Prize 2024.

Organic Synthesis and Medicinal Chemistry (OM-I-061)

Design and synthesis of unique 5-arylaminothiazoles with tunable photophysical properties

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The development of low molecular weight molecules with unique photophysical properties via novel synthetic routes is of great interest in the field of organic chemistry. In this study, we report the discovery of a new reaction between thioamide dianions, derived from secondary thioamides, and thioformamides, leading to the formation of 5-N-arylamino thiazoles. While numerous thiazoles have been synthesized by introducing diverse substituents at the three carbon positions of the thiazole ring, our compounds represent the first examples of thiazoles bearing nitrogen-containing substituents with electron-donating properties.

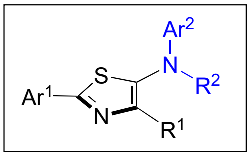
X-ray crystallographic analysis of selected compounds revealed a deviation of the 5-arylamino group from the thiazole ring. Nevertheless, the synthesized thiazoles exhibit fluorescence, with emission wavelengths tunable by modifying the substituents on the aromatic group attached to the nitrogen atom and at the 2-position of the thiazole ring.

As an alternative synthetic approach, we developed a three-step sequence starting from commercially available unsubstituted thiazole and 4-methylthiazole. This method involves Pd-catalyzed C–H functionalization at the 2-position, affording 2-arylthiazoles, followed by bromination to yield 2-aryl-5-bromothiazoles. The final step employs the Buchwald–Hartwig amination reaction to introduce the 5-arylamino moiety, enabling the synthesis of over 50 distinct 5-arylaminothiazoles.

Furthermore, we successfully incorporated pyridyl groups at the 2-position, producing thiazoles that exhibit halochromism and mechanofluorochromism. Additionally, thiazoles bearing functional groups reactive to thiols, amines, and hydrazine were evaluated as chemosensors for the detection of these analytes.

Density Functional Theory (DFT) calculations revealed that the highest occupied molecular orbital (HOMO) of the 5-arylaminothiazoles is primarily localized on the amino group, while the lowest unoccupied molecular orbital (LUMO) extends over the thiazole ring and the aromatic substituent at the 2-position.

In this presentation, we will discuss these findings in detail, including the synthetic strategies, structural characteristics, photophysical properties, and potential applications of our novel thiazoles.



5-*N*-arylaminothiazoles

Keywords: 5-arylaminothiazoles; DFT calculaion; photophysical properties; chemosensors

Toshiaki Murai was born in Osaka in 1957 and earned his Ph.D. in 1986 from Osaka University. He was a Research Associate at Gifu University (1983–1990), Associate Professor (1990–2001), and Professor (2001–2023). Since 2023, he has served as a Specially Appointed Professor at Gifu University. His research interests encompass organic chemistry and main group chemistry, and has been recognized with awards from the Society of Synthetic Organic Chemistry, Japan (SSOCJ) and the Chemical Society of Japan (CSJ).

Organic Synthesis and Medicinal Chemistry (OM-I-062)

Fluorine-substituted derivatives of γ-carbolines and carbazoles as a promising drug chemotype for the neurodegenerative disease treatment

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The search of effective drugs for the treatment of neurodegenerative diseases such as Alzheimer's disease, amyotrophic lateral sclerosis (ALS), Parkinson's disease is an extremely complex challenge. It is explained by both the multifactorial nature of most such pathologies and the difficulties in modeling CNS diseases *in vitro* and *in vivo*. The main modern trends in finding drugs for the neurodegenerative disease treatment are the targeted search for drugs that directly affect the pathogenesis of diseases, the creation of multi-target structures, and the repositioning of already known drugs [*Med. Res. Rev.* **2017**, 23, 13925].

Previously, neuroprotective activity of the domestic drug Dimebon (γ-carboline derivative) was discovered [*Lancet* **2008**, *372,* 207–215]. This compound has pronounced therapeutic properties in the 2nd phase of clinical trials in Alzheimer's disease patients. We carried out a targeted modification of the parent γ-carboline structure to find new neuroprotective properties in various cellular and animal models of neurodegenerative disorders [*Sci. Rep.* **2019**, *9*, e4873; *Sci. Rep.* **2022**, 12,12766; *CNS Neurosci. Ther.* **2021**, *27*, 765–775; *Russ. Chem. Bull.* **2023**, *72*, 130–147]. Pronounced antiaggregatory properties were found in a group of fluorinated derivatives in ALS models. Moreover, structures representing conjugates of fluorine-substituted carbazoles and aminoadamantanes demonstrated unique mitochondria stabilizing properties, which allows them to be considered as promising neuroprotective agents.

This work was supported by the Russian Ministry of Science and Education (Project 075-15-2024-638; Agreement No 12-223/MGp/2025).

Keywords: amyotrophic lateral sclerosis; Parkinson's disease; carboline; carbazole

Dr. Sergey Bachurin was born in 1953. He graduated Lomonosov Moscow State University (MSU) in 1975; in 1980 he received Ph.D. At present he is the Scientific Director of the Institute of Physiologically Active Compounds RAS. Main research activity related to the discovery and study of novel agents for neurodegenerative diseases treatment, in particular for Alzheimer's disease, ALS, parkinsonism. He is the full member of Russian Academy of Sciences (RAS).

Polymers and Bio-based Materials (PC-I-027)

Development of high-performance biodegradable biomass plastics and their deep-sea biodegradability

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To establish a sustainable material production system and preserve the beautiful global environment forever, it is desirable to develop “biomass plastics” that are made from renewable biomass instead of petroleum, and “biodegradable plastics” that are completely degraded into carbon dioxide and water by enzymes secreted by microorganisms in the environment.

This paper presents a series of studies on microbial polyesters and polysaccharide ester derivatives, including the synthesis of novel polymers, development of new processing techniques for high-performance films and fibers, elucidation of the relationship between structure and properties using synchrotron radiation, control of the rate of enzymatic degradation and environmental degradation. Furthermore, development of biodegradation initiation switch and self-degradable aliphatic polyesters in sea-water environment by embedding lipases via melt extrusion will be presented.

More recently, we succeeded to confirm microbial decomposition of representative biodegradable plastics (polyhydroxyalkanoates, biodegradable polyesters, and polysaccharide esters) at diverse deep-sea floor locations ranging in depth from 757 to 5552 m. The rate of degradation slowed with water depth. We analyzed the plastic-associated microbial communities by 16S rRNA gene amplicon sequencing and metagenomics. Several dominant microorganisms carried genes potentially encoding plastic-degrading enzymes such as polyhydroxyalkanoate depolymerases and cutinases/polyesterases. Our results confirm that biodegradable plastics can be degraded by the action of microorganisms on the deep-sea floor, although with much less efficiency than in coastal settings.

Keywords: polyhydroxyalkanoate; biodegradable polyesters; polysaccharide ester derivatives; biodegradation initiation function; deep-sea biodegradation

Dr. Tadahisa Iwata is a Professor at The University of Tokyo, specializing in biodegradable and bio-based polymers as well as polymer structure. He earned his PhD from Kyoto University in 1994 and gained research experience at CERMAV-CNRS in France and RIKEN Institute in Japan. Dr. Iwata has received multiple prestigious awards, including the German Innovation Award (2009) and the Japanese Minister of Education, Culture, Sports, Science and Technology Award (2020), recognizing his impactful contributions to polymer science and sustainable materials.

Polymers and Bio-based Materials (PC-I-032)

Melt electrowriting 3D printing of biobased polymers

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Melt electrowriting (MEW) is an advanced 3D printing technique used to fabricate high-resolution tissue engineering scaffolds. Although MEW has been successfully applied to various biobased polymers, most exhibit low printability, except for polycaprolactone. In this context, we developed several novel MEW systems capable of printing a broader range of biobased polymers, including poly(L-lactic acid), poly(glycolic-co-lactic acid), and poly(glycolic acid). A comprehensive protocol for evaluating the printability of these materials was established, incorporating metrics such as jet lag angle, Taylor cone area, sample weight, viscosity, and molecular weight over extended printing periods. Furthermore, we systematically investigated the mechanical properties, toxicity, and hydrolysis behavior of these polymers. The potential application of these scaffolds in bone tissue repair and their prospects in broader tissue engineering and regenerative medicine are also explored.

Keywords: 3D printing; electrospinning; printability; tissue engineering

Dr. Huaizhong Xu, born in 1989, earned his PhD in Engineering from Kyoto Institute of Technology in 2018. He is an associate professor leading a research group focused on advanced functional fibers and 3D printing technologies. With a background in textile materials, he developed Electro-centrifugal spinning technology and specializes in Melt Electrowriting (MEW). Xu has published over 50 articles, contributed to technology development, and is recognized for his interdisciplinary expertise.

Physical and Theoretical Chemistry (PT-I-015)

Understanding peptide self-assembly: Bionanostructures and antimicrobial peptides

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Self-assembly of peptide-based building blocks has been shown to be useful in constructing artificial bionanostructures. Computational studies can provide useful insights in studying the principles governing the formation of self-assembled nanostructures. We performed molecular dynamics simulations on the self-assembled supramolecular nanotube constructed by amphiphiles with a bent-shaped rod as a building block. By systematically examining small aggregates composed of several molecules to the fully constructed nanotube, we identified optimal structures consistent with experimental findings. Research on antimicrobial peptides (AMPs) has been conducted as a solution to overcome the problem of antibiotic resistance. We conducted molecular dynamics simulations for two heterogeneous aggregates of melittin-indolicidin and pexiganan-indolicidin to observe their structures in the solution phase and their interactions with the lipid membrane. It was found that the amino acid residues forming the surface of the AMP aggregate show differential binding strengths to different lipid species forming the lipid membrane, thereby disrupting the membrane in a way that weakens its integrity, providing insight into the basic principle of the synergy effect of AMPs.

Keywords: self-assembly; peptides; bionanostructures; AMP; MD simulations

Seokmin Shin received a bachelor's degree with Honors in 1985 and a master's degree in 1987 from Seoul National University. He continued his graduate studies at the University of Chicago, where he obtained a PhD under the supervision of Stuart A. Rice. In 1995, he joined Seoul National University as a faculty member, where he currently holds the position of Professor of Chemistry. He served as the President of the Korean Chemical Society during 2022~2023. His research primarily centers on studying the dynamical processes involved in the chemical changes that lead to specific functions of molecular systems.

Physical and Theoretical Chemistry (PT-I-017)

Mechanistic study of thioester hydrolysis catalyzed by boric acid and its derivatives

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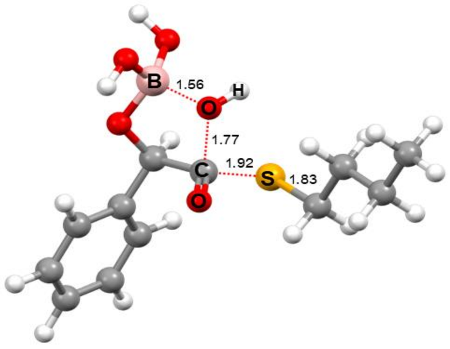
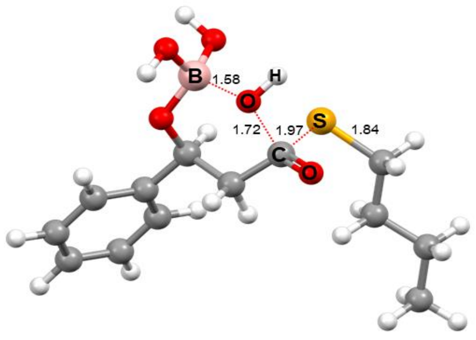
Thioesters play a crucial role as intermediates in peptide and protein synthesis. In particular, thioester hydrolysis is a key step in their chemical synthesis and requires effective catalysts. Boric acid has been proposed as a catalyst for thioester hydrolysis. We have developed a novel additive, 2-mercaptophenylboronic acid (2-MPBA), for peptide thioester hydrolysis under mild conditions. However, the detailed reaction mechanisms of boric acid- and 2-MPBA-catalyzed hydrolysis remain unclear. Understanding these mechanisms could help in the design of more efficient catalysts. In this study, we investigated the reaction mechanisms of thioester hydrolysis catalyzed by boric acid and 2-MPBA using DFT calculations. Our results revealed that for both α-hydroxy thioester (**1**) and β-hydroxy thioester (**2**), hydrolysis occurs in two steps: the formation of butanethiol (BuSH) and carboxylate. The rate-determining step involves B–O bond cleavage, OH migration, and C–S bond cleavage. Notably, the transition state of substrate **1** forms a five-membered ring with boron, an OH group, and a carbonyl group, whereas substrate **2** forms a six-membered ring, which accelerates hydrolysis. Furthermore, 2-MPBA catalysis follows a mechanism similar to that of boric acid, involving methanethiolate (MeS^-) and carboxylate formation.

Keywords: thioester; hydrolysis; mechanism; boric acid; 2-mercaptophenylboronic acid



Five-membered ring TS of substrate 1



Six-membered ring TS of substrate 2

Manussada Ratanasak received her Ph.D. in Nano Science and Technology from Chulalongkorn University in 2016. She subsequently joined the Institute for Catalysis (CAT) at Hokkaido University as a postdoctoral researcher, working with Prof. Jun-ya Hasegawa until 2024. She is currently a researcher in Prof. Yasuteru Shigeta's group at the Center for Computational Sciences, University of Tsukuba. Her research focuses on computational studies of catalytic reaction mechanisms, organocatalysis in organic synthesis, organometallic catalysis for asymmetric synthesis, photocatalytic systems, catalyst design using QSAR/QSPR approaches, enzymatic reaction mechanisms, and materials science applications.

Physical and Theoretical Chemistry (PT-I-018)

Software development and application for material design based on the statistical mechanics theory of liquids

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Biological environments are composed of complex mixtures of water, electrolytes, proteins, lipids, and various other biomolecules. To design biocompatible materials that function effectively in such environments, it is essential to account for the intricate physicochemical properties of these multi-component solutions. Traditional simulation approaches often face challenges when trying to capture solvent effects at molecular resolution, especially in heterogeneous and biologically relevant conditions.

To address this, we have developed software based on the three-dimensional reference interaction site model (3D-RISM), a statistical mechanics theory of molecular solvation, referred as the reference interaction site model integrated calculator (RISMiCal). The 3D-RISM theory enables the efficient and accurate prediction of solvation structures and thermodynamic properties by solving integral equations for solvent distribution functions around solutes. Our implementation focuses on biomolecular systems, allowing for the analysis of solvation and interactions of proteins, polymers, and other macromolecules in solution.

This software provides a powerful platform for understanding the structure-function relationship of biomolecules in complex solvents and has applications in material design, drug discovery, and biotechnology. In this presentation, we will introduce the theoretical background and capabilities of the software, highlighting recent advancements in methodology, including improvements in numerical solvers, hybrid approaches with molecular dynamics, and enhanced sampling techniques.

Furthermore, we will discuss recent developments that integrate 3D-RISM theory with machine learning methods. By combining physics-based solvation theory with data-driven models, we aim to accelerate the prediction and screening of material properties, opening new avenues in the design of smart, adaptive, and biocompatible materials.

Keywords: solvation theory; 3D-RISM; software

Prof. Norio Yoshida, born in 1973, is a Professor at the Graduate School of Informatics, Nagoya University. He earned his degrees in science, specializing in theoretical and computational molecular science. His research focuses on the molecular theory of solvation, aiming to understand solvation phenomena at the molecular level through advanced computational methods.

Oxidative upcycling of polyethylene waste into dicarboxylic acid

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Polyethylene (PE) constitutes 36% of waste plastics by weight and poses significant environmental challenges due to its chemically stable C–C backbone, which resists natural decomposition. Chemical upcycling of PE into valuable products has thus emerged as a promising strategy in plastic recycling. Our recent research has developed a catalytic oxidation process that transforms waste PE into long-chain dicarboxylic acids under mild conditions (160 °C, 1.5 MPa air). These acids are crucial for high-grade lubricants, coatings, and synthetic nylon. We have successfully designed both noble and non-noble metal catalyst systems (e.g. Ru/TiO_2, TS-1, ZSM-5, etc), which demonstrate excellent performance across various PE sources, including recycled plastics. This innovative approach not only offers a sustainable solution for PE waste upcycling but also holds potential for extending to other high-value chemicals and plastic types.

Keywords: plastic waste; upcycling; catalytic oxidation; mild conditions; dicarboxylic acid

Dr. Lei Huang is a Full Professor at Research Center of Nano Science and Technology, Shanghai University. His research interest focuses on nanomaterial design for environmental catalysis and gas sensors. He received his Ph.D. from South China University of Technology (2009), with research experience at the University of Washington (2007-2008). He completed a postdoctoral fellowship at Dalian Institute of Chemical Physics, CAS (2010). He was promoted as an Associate Professor in 2013 and full Professor at Shanghai University in 2024. He has published 80+ papers in Angew. Chem. Int. Ed., J Catal., Appl. Catal. B, etc. with 4,000+ citations.

Physical and Theoretical Chemistry (PT-I-021)

Sunlight-driven detoxification of harmful antibiotics in the environment by using metal oxide photocatalysts

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In this talk, the preparation, characterization and application of sunlight-active photocatalysts for removal of antibiotics will be presented. Firstly, magnetic Fe_3O_4/ZnO photocatalyst was prepared using an ultrasonic route for removal of tetracycline (TC) antibiotic. The Fe_3O_4/ZnO provided the lowest photoluminescence intensity indicating the greatest effective charge separation efficiency. The efficiency of 100% toward removal of TC antibiotic was reported after 20 min. The magnetic photocatalyst still displays high photocatalytic performance after the fifth cycle. Secondly, the ternary Fe_2O_3/g-C_3N_4/ZnO photocatalyst was constructed using an ultrasonic method. The prepared photocatalyst was used for sunlight-active photodegradation of tetracycline (TC) antibiotic in aqueous solution. The 0.10%wtFe_2O_3/g-C_3N_4/ZnO (denoted as 0.10Fe_2O_3/g-C_3N_4/ZnO) exhibited the lowest fluorescence intensity, implying the lowest charge recombination rate among all prepared samples. The result correlates well with the highest photocatalytic performance found in the 0.10 Fe_2O_3/g-C_3N_4/ZnO. Great photoactivity of 100% was achieved after 4 h under natural sunlight illumination attributing to the maximum charge separation efficiency of the sample, compared to other synthesized photocatalysts. The photodegradation of TC correlates well with the first-order reaction. The rate constant of 0.03530 min^{-1} was reported. The ternary heterostructure still shows its enhanced photoactivity after the fifth run. The trapping experiment shows that the photo-created electrons play a huge role in TC removal. The present work shows the new avenue to generate the three-component heterostructure for degradation of harmful TC in the environment.

Keywords: ZnO; heterostructures; magnetically separable; sunlight; tetracycline

Dr. Suwat Nanan (b 1978) received his PhD in Chemistry from University of Leeds, UK in 2009. He was promoted to Assistant Professor and Associate Professor in 2015 and 2020, respectively. His research interests focus on semiconducting photocatalysts for environmental protection including the creation of sunlight driven photocatalysts for removal of organic pollutants such as organic dyes, antibiotics, and insecticides in wastewater.

Physical and Theoretical Chemistry (PT-I-022)

Zeolite-based strategies for CO_2 capture and methanation

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The rising concentration of atmospheric carbon dioxide (CO_2) is a major driver of global warming and necessitates the development of efficient capture and utilization technologies. This presentation summarizes our recent work on zeolite-based materials for CO_2 adsorption and methanation, highlighting the relationship between material structure and performance. First, high-purity silica was extracted from sugarcane bagasse ash using a direct alkaline method and used to synthesize zeolite NaA. The resulting adsorbents showed CO_2 adsorption capacities of 4.1–4.3 mmol/g, comparable to commercial NaA. Second, nanosized zeolite Y (NaY) was synthesized via a template-free hydrothermal method, where variations in aluminum source and water content led to significant changes in particle size (50–100 nm), crystallinity, and adsorption capacity. Smaller particles provided greater surface area and higher CO_2 uptake. Third, NaY was composited with acid-treated bamboo wood, followed by carbonization to produce zeolite-carbon composites. The composite with nanosized NaY exhibited the highest CO_2 adsorption capacity per gram of zeolite, attributed to better dispersion and diffusion within the carbon matrix. Finally, zeolite-supported nickel (Ni) catalysts were evaluated for CO_2 methanation. Three supports (LTA, ANA, and ZSM-5) were compared, and their physicochemical properties were characterized using in situ X-ray absorption spectroscopy (XAS) connected online with gas chromatography (GC) and mass spectrometry (MS); X-ray diffraction (XRD), and nitrogen sorption techniques. The 5 wt% Ni/LTA catalyst showed the highest CH_4 selectivity and CO_2 conversion. Operando XAS-MS revealed that the Ni reducibility, influenced by the zeolite support, played a key role in catalytic activity. These results demonstrate that both CO_2 adsorption and methanation performance can be enhanced by tuning zeolite composition, morphology, and support functionality. The findings offer insights into the rational design of multifunctional zeolite-based materials for sustainable CO_2 management.

Keywords: zeolite-based materials; CO_2 adsorption; CO_2 methanation; sustainable synthesis; structure–performance relationship

Jatuporn Wittayakun received his Ph.D. from the University of Wisconsin-Madison. He is a full professor in chemistry and the head of the Materials Chemistry Research Center for Sustainability in Energy and Environment at Suranaree University of Technology (SUT). His research interest is in the synthesis and modification of porous materials, particularly zeolites, for adsorption and heterogeneous catalysis. He recently received the 2024 Distinguished Chemist (Inorganic Chemistry) award from the Chemical Society of Thailand.

Physical and Theoretical Chemistry (PT-I-023)

Understanding 3d transition metal carbonyl bonding from multistate coupling

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Transition metal (TM) carbonyls are fundamental chemical complexes in many important biological and catalytic processes. The binding of early and late 3d transition metal atoms with carbonyl was reported to change the spin state. However, till now, no study has evaluated the spin-orbit (SO) effect along the whole association pathway of any TM-CO bond. Using multireference calculations with SO interaction, we calculated the association potential energy curve (PEC) for multiple electronic and spin states for Ni + CO → NiCO, Co + CO → CoCO, and Fe + CO → FeCO. SO multireference calculations showed that SO results in a spin barrier of a few tenths of eV along the TM-CO association pathway. These calculations provide a new understanding of the overlooked yet important effect of the spin barrier on the association process, which can change the association rate by several orders of magnitude.

Secondly, we compared these multistate results with the calculations by density functional theory (DFT) methods and found that the binding energy can be reproduced using hybrid functionals. Furthermore, details concerning basis set dependence and how effective core potential can affect the spin state energies will be discussed in the talk.

Keywords: spin state; spin-orbit interaction; density functional theory; multireference configuration interaction; effective core potential

Kaito Takahashi obtained his Ph.D. degree from Keio University under the supervision of Prof. Satoshi Yabushita in 2005. He worked at the Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, from 2009 to 2024. He then moved to Sirindhorn International Institute of Technology, Thammasat University as a lecturer. His scientific interests for the past few years have been to theoretically understand properties that control reactions and to simulate experimental observables such as rate coefficients, IR, Raman, UV and X-ray spectra.

Physical and Theoretical Chemistry (PT-I-024)

Rational design of 2D materials for hydrogen storage: Tuning metal-adsorbate interactions via defect engineering

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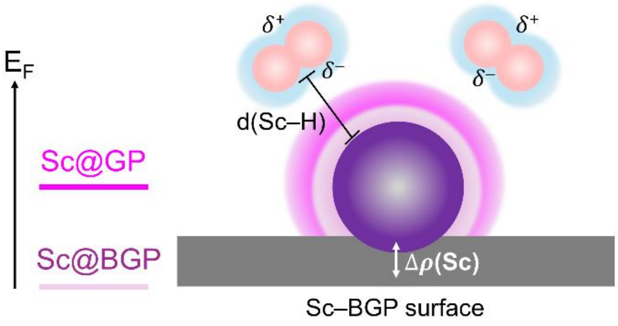
The rational design of two-dimensional (2D) materials for hydrogen storage relies on precise control over metal-adsorbate interactions, which can be tuned through defect engineering and electronic-structure modifications. In this presentation, I will discuss how we used computational tools to systematically explore metal decoration and defect introduction that influences hydrogen adsorption on boron-carbon-nitride (B_4CN_3) and boron-doped graphene. Our results reveal that while alkali and alkaline earth metals exhibit weak physisorption, 3d transition metals—particularly scandium (Sc)—enable stronger Kubas-type interactions. However, excessive metal aggregation and weak adsorption energies often hinder practical storage performance. To address this, we introduce controlled vacancy defects, with carbon vacancies in B_4CN_3 effectively shifting the Fermi level, strengthening hydrogen binding, and increasing temperatures. Similarly, boron doping in graphene enhances Sc stability, preventing aggregation and tuning hydrogen adsorption from Kubas to dipole-induced physisorption. Ab initio molecular dynamics simulations further identify Mg, Ca, and Sc as promising candidates for pristine B_4CN_3, while Li, Na, K, and Ca show potential for defective B_4CN_3.

Keywords: H_2 storage; density functional theory; 2-dimensional materials; defect engineering.



*Dr. Suthirakun is an associate professor at School of Chemistry, Suranaree University of Technology. He received his PhD (2013) in Chemical Engineering from University of South Carolina and spent 2 years as a scientist at IHPC, A*STAR, Singapore. His research group used computational tools, based on first-principles calculations, to obtain better understanding of structure-performance relationships of functional materials including energy materials and heterogenesous catalysis.*

Physical and Theoretical Chemistry (PT-I-025)

Excited state intramolecular proton transfer (ESIPT) from principal photophysics to the development of new chromophores and applications in fluorescent probes and luminescent materials

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Chromophores possessing excited-state intramolecular proton transfer (ESIPT) are of great important in the past decades because of their desirable unique photophysical properties which can be used in various applications ranging from optoelectronic devices such as light emitting diodes and laser dyes, molecular switching to fluorescent probes both in chemical and biological systems. Therefore, the development of new chromophores based on the ESIPT process have been intensively developed using combined experimental approach and theoretical study. The identification of how structural modifications controlling their optical properties driven by ESIPT process and solvent media affecting their fluorescent emission are of great importance. Thus, our group is interested in studying several aspects in terms of electronic properties and ESIPT process through the computational chemistry as an effective tool. Moreover, the systemic study and molecular screening using certain criteria will be carried out to provide the best candidates for applications in fluorescent probes and light emitting diodes. The identification of the fundamental of conformational aspects of important ESIPT molecules in non-polar and polar solvents. These aspects include: (1) the molecular and electronic structures of the dyes, especially the multiple emission character from single proton transfer or double proton transfer; (2) the spectral tuning and (3) the sensitivity of ESIPT process to the environmental factors (solvent effect). The results obtained are useful for experimentalists in molecular designing high fluorescence efficiency and long lifetime of ESIPT molecules towards fluorescent molecular probes and luminescent materials. Finally, the selected of designed compounds that pass the important criteria are recommended to synthesize and test for application uses in fluorescent probes and solid-state emitters based on ESIPT process.

Keywords: excited-state intramolecular proton transfer; computational chemistry; fluorescent molecular probe; luminescent material

Dr. Nawee Kungwan obtained his PhD degree in Chemistry under the direction of Prof. Thanh N. Troung in 2007 from the University of Utah, USA. He was a lecturer in the Department of Chemistry, Chiang Mai University in 2007 and a postdoctoral researcher in 2009 at University of Vienna. He was promoted to assistant professor and associate professor in 2014 and 2019, respectively. His research interests focus on computational chemistry of light emitting materials, catalyst for ring-opening polymerization, catalytic materials for upgrading bio-oils, excited-state proton transfer and molecular design for fluorescent probes.

Physical and Theoretical Chemistry (PT-I-026)

The Thailand public energy materials database 2.0 (TPEM 2.0) for catalyst and energy materials design

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[3]*Research Center for Theoretical Simulation and Applied Research in Bioscience and Sensing, Walailak University, Nakhon Si Thammarat 80160, Thailand*
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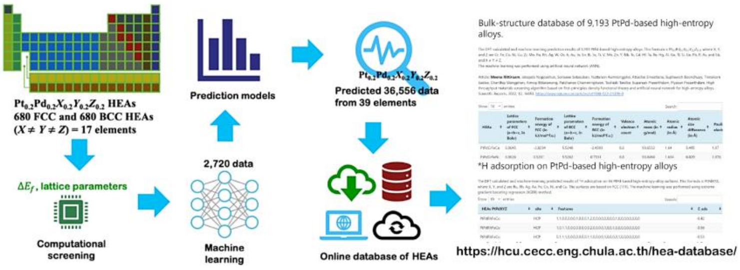
The Thailand Public Energy Materials Database 2.0 (TPEM2.0) is designed to support researchers in the field of energy materials design, including catalytic materials, energy storage materials, and hydrogen storage materials. This database integrates first-principles calculations based on density functional theory (DFT) with machine learning techniques to provide tailored materials properties as descriptors for materials design. For example, in electrocatalyst development, adsorbate binding energy serves as a key descriptor, ensuring that catalytic materials exhibit neither excessively strong nor weak adsorption, thereby optimizing activity for target reactions. A distinctive feature of TPEM2.0 is its inclusion of high-entropy materials (HEM), a promising class of materials with diverse applications in high-performance alloys, battery electrodes, and heterogeneous catalysis. Supported by the National Research Council of Thailand (NRCT) and Chulalongkorn University, this project also aims to empower young researchers in low- and middle-income countries, enabling them to initiate materials science and engineering research based on reliable computational data.

Keywords: heterogeneous catalysis; hydrogen storage; high-entropy materials



Supareak is the Director of Center of Excellence on Catalysis and Catalytic Reaction Engineering (CECC), the Principal Investigator of the High-Performance Computing Unit (CECC-HCU), and an Associate Professor at the Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University. He received his Ph.D. (Chemical Engineering) from Texas A&M University in 2018. His research focuses on computational heterogeneous catalyst design using density functional theory, microkinetic modeling, and machine learning. In 2017, he received the Richard J. Kokes Award from the North American Catalysis Society (NACS), USA.

Physical and Theoretical Chemistry (PT-I-027)

Machine learning-based QSAR application on ebsulfur and ebselen derivatives for SAR-CoV-2 main targeting for COVID-19

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Ebsulfur and ebselen derivatives that were proven to be potent inhibitors against the main protease (M^{Pro}) of SARS-CoV-2 which is an essential enzyme for viral replication were chosen to study the quantitative structure-activity relationship (QSAR) analysis using a classical multiple linear regression (MLR) and a machine learning approach of random forest (RF) and artificial neural network (ANN) in order to find the relationship between molecular structural properties and biological inhibitory activities. With the statistical criteria, the R^2 values of MLR, RF, and ANN models for the training set were 0.83, 0.82, and 0.92, respectively. The RMSE values of the test were considered for model evaluation, and the results were 0.27, 0.18, and 0.09 for MLR, RF, and ANN models, respectively. Therefore, the ANN model was the best-obtained model for predicting the M^{Pro} inhibitory activity of thirteen new synthetic ebselen analogs that haven't tested the biological assay before. Notably, our predicted inhibitory activities against SARS-CoV-2 were then examined using enzyme-based assays and cytotoxicity tests, which found that compound P8 resulted in a good potential candidate for SARS-CoV-2 M^{Pro} inhibitory activity. Furthermore, the molecular dynamics simulations were performed to study the dynamic interaction of ligand and binding site; the results showed a binding pathway and mechanism of compound P8 with key residues surrounding the active site of SARS-CoV-2 M^{Pro}, which is useful for further development of ebselen derivatives.

Keywords: ebselen and ebsulfur derivatives; SARS-CoV-2 inhibitory activity; QSAR; machine learning; LB-PaCS-MD

Phornphimon Maitarad is an Associate Professor at Shanghai University, specializing in computational chemistry. She earned her Ph.D. from Kasetsart University in 2008. Her research focuses on catalyst design using DFT and computer-aided drug design (CADD) for SARS-CoV-2, combining virtual screening, molecular docking, and dynamics simulations.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-005)

Red light uncaging reactions of organorhodium phthalocyanine complexes: Experimental and theoretical insights

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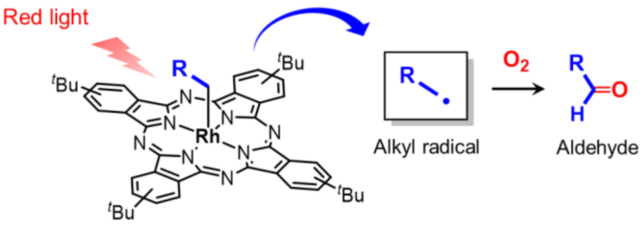
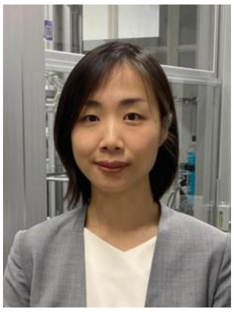
Photodynamic therapy (PDT) has gained significant attention as a minimally invasive cancer treatment due to its tumor-selective cytotoxic effects. However, since PDT relies on the photochemical generation of reactive oxygen species (ROS) by photosensitizers, effective treatment of tumor cells in hypoxic environments, where oxygen tension is low, remains a challenge. To address this issue, we have developed a novel red light uncaging reaction using organorhodium(III) phthalocyanine complexes. These complexes release reactive carbon species (alkyl radicals and aldehydes) derived from the axial ligands in addition to ROS, enabling tumor cell attack independent of the oxygen environment.

A series of rhodium phthalocyanine complexes bearing various alkyl ligands was synthesized, and their uncaging abilities were evaluated under red light irradiation. As a result, complexes with simple alkyl ligands induced metal-carbon bond activation under irradiation with a nanosecond pulsed laser of red light, whereas complexes with benzyl or allyl ligands induced similar activation even under irradiation with continuous-wave red light. Experimental and theoretical analyses suggested that the former reaction proceeded via stepwise two-photon excitation, while the latter was induced by single-photon excitation.

In this presentation, the details of the photophysical, photochemical, and photodynamic properties of the complexes will be discussed.

Keywords: rhodium; phthalocyanine; photouncaging





Kei Murata was born in 1985 in Tokyo, Japan. She received her Ph.D. in 2013 from Tokyo Institute of Technology under the supervision of Prof. Munetaka Akita. Afterward, she joined the research group of Prof. Kazuyuki Ishii at the University of Tokyo. She is currently serving as the RIKEN ECL unit leader at RIKEN. Her research interests focus on the development of new photochemical reactions of organometallic complexes. She received the Chemical Society of Japan Award for Outstanding Young Women Chemists in 2023.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-006)

Introduction to the Thailand-Japan Bilateral Symposium: Advancing synchrotron science through experimental and computational chemistry synergy

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The Scope of the one-and-half-day Thailand-Japan bilateral symposium is as follows: “Theoretical and computational chemistry are rapidly advancing, while experimental methods remain central. In addition to traditional experimental methods, quantum beam sciences, including advanced synchrotron science, are becoming essential tools for chemistry, material sciences, and engineering. During this one-and-a-half-day symposium, distinguished speakers will highlight the excellent collaborative experiences between theoretical/computational and experimental chemists, as well as synchrotron scientists from Thailand and Japan. They will also discuss ways to enhance future collaborations, particularly in contributing to a sustainable society.”

I will present a summary of my research related to homogeneous catalysis, along with examples of research collaborations between my group and Thai chemistry groups. Additionally, I will showcase the quantum beam sciences.

Keywords: synchrotron science; Thailand; Japan; theoretical and computational chemistry; homogeneous catalysis

Seiji Mori obtained his Ph.D. from the University of Tokyo in 1998. After completing postdoctoral fellowships at Emory University and at Kyoto University, he became an assistant professor of environmental science at Ibaraki University in 2000. He was promoted to associate professor in 2001 and full professor of chemistry in 2012. He served as assistant vice president from 2015 to 2017 and as director of the Institute of Quantum Beam Science from 2022 to 2025. His research focuses on the computational chemistry of organic, organometallic, and biological reaction mechanisms.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-008)

Reaction mechanism and catalyst design of transition metal complexes

Ray Miyazaki,[1] Sarinya Hadsadee,[1] Manasada Ratanasak,[1,2] Jun-ya Hasegawa[1,*]
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In the presentation, a summary of our recent research activity on the transition metal catalyzed reactions will be presented. The first topic is Ni-catalyzed benzofuran synthesis. Reductive elimination often becomes rate-determining step and thermodynamically unfavorable. The coordination of a new substrate changes this step being exergonic and also regulates the course of the reaction. In the second topic, a halogen trend in the reactivity observed in a Ru-catalyzed dehydrative cyclization will be discussed. A decomposition analysis revealed that the halogen bond between catalyst and substrate destabilizes the reactant state. As a result, the activation energy decreases as the halogen bond is stronger. The third topic is catalyst design for the Ni-catalyzed H_2 production/oxidation. Depending on the oxidation number, the Ni complex in singlet state changes the relative stability of tetrahedral vs octahedral coordination structures. This point is useful for the ligand design to be used for H_2 production/oxidation. With the Dubois's Ni catalyst, a sterically demanding ligand is suitable for H_2 oxidation, while a rigid planer ligand modifies the catalyst being better suited to H_2 production.

Keywords: DFT calculation; reaction mechanism; catalyst design; transition metal complexes

Jun-ya Hasegawa

1998 PhD from Graduate School of Engineering, Kyoto University
1998 Postdoctoral Researcher, Lund University, 1999 Assistant Professor, Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, 2011-2012 Associate Professor, Fukui Institute for Fundamental Chemistry, Kyoto University, 2012- Professor, Institute for Catalysis, Hokkaido University

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-009)

Innovative battery technologies for sustainable energy: Integrating experimental and DFT insights

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With the growing global demand for sustainable energy solutions, the development of next-generation battery technologies has become critical. Density Functional Theory (DFT) has revolutionized materials research by providing atomic-scale insights that accelerate the design and optimization of energy materials. This talk presents a synergistic approach combining DFT simulations and experimental validation to advance battery technologies for renewable energy integration. Key computational methodologies enabling precise predictions of material properties will be discussed, alongside case studies demonstrating breakthroughs in catalyst design and energy storage materials. Finally, challenges and future research directions will be highlighted, emphasizing the essential role of computational-experimental collaboration in driving innovations for a more sustainable energy future.

Keywords: sustainability; energy materials; battery technologies; DFT; catalysis

Siriporn Jungsuttiwong received her Ph.D. in chemistry from Kasetsart University. She is currently a full professor at the Department of Chemistry, Ubon Ratchathani University. Her research interests include computational chemistry, with a focus on the catalytic reactivity of nanomaterials. She was an awardee of the 2017 TRF-OHEC-Scopus Researcher Awards (Physical Sciences) and the 2019 TRF-OHEC-Clarivate Analytics Research Excellence Award.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-010)

Towards sustainable energy solutions: Novel materials and architectures for zinc-air batteries

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The growing demand for sustainable energy solutions necessitates the development of efficient and scalable energy storage technologies. Rechargeable zinc-air batteries (ZABs) have emerged as promising candidates for grid-scale energy storage due to their high energy density, cost-effectiveness, and environmental sustainability. However, their widespread adoption is hindered by challenges related to sluggish oxygen reduction (ORR) and oxygen evolution (OER) reactions, as well as the stability of air electrodes during long-term cycling. This study presents recent advancements in the design and development of bifunctional electrocatalysts and engineered electrode architectures to address these limitations. We highlight the synthesis of metal-organic framework (MOF)-derived defect-rich spinel ferrites supported on nitrogen-doped carbon matrices, which exhibit superior ORR activity through enhanced oxygen adsorption and electron transfer kinetics. Additionally, innovative OER catalysts based on transition metal oxides and their composites are explored to improve charge transfer efficiency and catalytic stability. Beyond catalyst development, electrode structuring plays a crucial role in optimizing battery performance. Strategies such as hierarchical porosity control, gas diffusion layer modification, and scalable electrode fabrication techniques are discussed in relation to enhancing mass transport, mechanical integrity, and electrochemical durability. Furthermore, the integration of tri-electrode configurations in ZABs is examined as a means of decoupling ORR and OER processes, thereby mitigating electrode degradation and extending cycle life. These advancements collectively contribute to more robust and high-performance zinc-air batteries, paving the way for their practical implementation in large-scale renewable energy storage systems. This work aligns with the theme of "Responsible Chemical Sciences for World Sustainability" by promoting electrochemical solutions that enable clean energy transitions and long-duration energy storage. The insights from this research offer a pathway toward achieving a more resilient and sustainable energy future.

Keywords: oxygen electrocatalysts; tri-electrode design; large scale; dendrite; wettability

Soorathep Kheawhom (b. 1976) is an Associate Professor of Chemical Engineering at Chulalongkorn University, Thailand. He earned his Ph.D. from the University of Tokyo in 2004. His research focuses on zinc-based energy storage systems, with over 250 publications and patented innovations. He has received Gold Medals at the International Exhibition of Inventions Geneva and actively collaborates on sustainable energy solutions.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-011)

Nano-structured heterogeneous catalysts for organic syntheses

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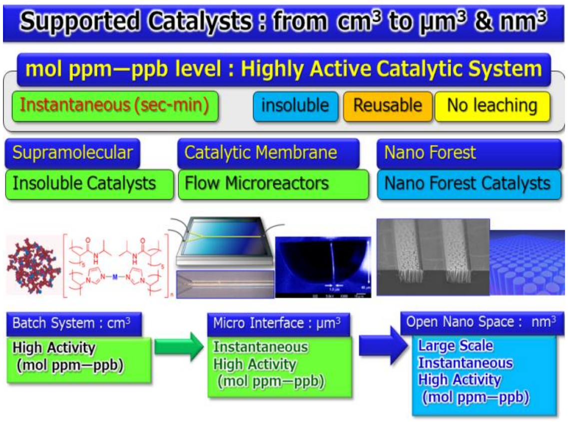
Our research focuses on developing highly efficient and recyclable catalysts for organic transformations. We aim to unlock the full potential of catalysts to enable previously unexplored reactions. Additionally, we analyze the effects of light and microwave irradiation on catalytic performance and explore reactions that benefit from these conditions. A key aspect of our work is designing catalysts tailored for environmentally friendly processes, promoting sustainable chemistry.

To achieve these goals, we employ various strategies. First, we synthesize self-organized catalysts by integrating polymer ligands and metal species, ensuring precise structural control [*JACS Au* **2021**, *1*, 2080, and references cited therein]. Second, we develop spatial catalysts by incorporating micro/nanomaterials into catalytic matrices, significantly enhancing efficiency and selectivity [*ACS Catal.* **2020**, *10*, 2148]. Finally, we explore electromagnetic wave-activated catalysts, which utilize light or microwave irradiation to drive catalytic transformations [*ACS Catal.* **2023**, *13*, 12665].

In this lecture, I will present case studies from our recent work, demonstrating the effectiveness of these approaches in advancing catalytic science.

Keywords: self-organized catalysts; nano-structured catalysts; XANES; EXAFS; electromagnetic wave-activated catalysts



Yoichi M. A. Yamada
Education: The University of Tokyo (Ph.D., 1999).
Work: Team Leader, RIKEN Center for Sustainable Resource Science (2018–present). Coordinate Professor, Saitama University; Visiting Professor, Shizuoka University; Visiting Professor, Kyushu University; Visiting Professor, Institute of Science Tokyo; Visiting Professor, National Chung Hsing University, Taiwan
Field of research: Organic and Catalytic Chemistry, Nano Chemistry

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-012)

Nickel or palladium-catalyzed decarbonylative transformations of acyl fluorides and chlorides

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Given the growing concerns about environmental sustainability, carboxylic acids—naturally abundant and readily available—are in high demand as alternative carbon feedstocks. In recent years, we have intensively studied the decarbonylative transformations of acyl fluorides, a key derivative of carboxylic acids. Since Schoenebeck's groundbreaking report on palladium-catalyzed decarbonylative trifluoromethylation of acyl fluorides in 2018, we have extensively explored various Ni-catalyzed decarbonylative transformations of both acyl fluorides and chlorides. Under optimal conditions, these reactions have demonstrated excellent functional group tolerance, accommodating cyano, halides (F and Cl), ketones, and esters.

We have developed an efficient and practical method for nickel-catalyzed decarbonylative cyanation of acyl chlorides using TMSCN, successfully converting a wide range of acyl chlorides into nitriles with good to excellent yields. Mechanistic studies suggest that PPh_3 ligands play a crucial role in facilitating both the decarbonylation and reductive elimination steps. Interestingly, when the stronger electron-donating ligand PEt_3 was employed, the oxidative adduct exhibited reduced CO release in the absence of TMSCN, allowing us to isolate an acyl–Ni complex as an intermediate. Conversely, in the presence of TMSCN, transmetalation occurred smoothly prior to decarbonylation. Additionally, our recently developed decarbonylative carbon–halogen bond-forming reaction, further expanding the scope of decarbonylative functionalization will also be discussed.

Keywords: acyl fluoride; decarbonylation; nickel; palladium; carboxylic acid derivatives

Prof. Yasushi Nishihara was born in Hiroshima, Japan in 1968. He earned his B.S. degree from Hiroshima University in 1992 and received his Ph.D. in 1997 from the Graduate University for Advanced Studies. In 1996, he became an Assistant Professor at Tokyo Institute of Technology, before moving to Okayama University in 2004 as an Associate Professor. He was promoted to Full Professor in 2010. His current research interests focus on organic synthesis mediated and/or catalyzed by organometallic compounds, as well as their applications in functional materials.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-013)

Pd-catalyzed synthesis of allenes: Experimental observations and theoretical rationale

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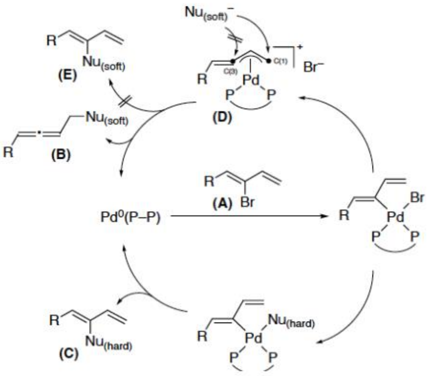
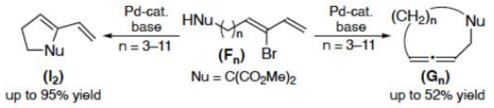
Palladium-catalyzed nucleophilic substitution of 2-bromo-1,3-dienes **A** displays two distinctive reaction modes depending on the nature of a nucleophile. While the reaction with a soft nucleophile provides allenic product **B**, conjugate diene **C** is a unique product from the reaction with a hard nucleophile. A key intermediate of the reactions is an alkylidene-π-allylpalladium species **D**. A soft nucleophile attacks at sp^3 C(1)-terminal of the η^3-butadien-3-yl moiety in **D** with a complete regioselection, and formation of conjugate diene **E** has never been detected so far. Recently, we have examined an intramolecular variant of this reaction using a series of ω-nucleophile-tethered-3-bromo-1,3-dienes $\mathbf{F_n}$ ($n = 2$-11). The trends of the regioselectivity in the palladium-catalyzed reaction of $\mathbf{F_n}$ ($n \geq 3$) were similar to those of the intermolecular process. On the other hand, the reaction of $\mathbf{F_2}$ showed completely different regiochemistry giving the corresponding vinylcyclopentene derivatives $\mathbf{I_2}$ predominantly. This is the first (and so far, the only) example in which a soft nucleophile attacks at the internal sp^2 C(3) carbon in an alkylidene-π-allylpalladium intermediate. The Surawatanawong group in Thailand conducted the *ab initio* calculations on the palladium-catalyzed processes and rationalized the two key regioselective issues in the reactions: (i) why the nucleophilic attack of a soft nucleophile takes place at C(1) in **D** predominantly not at C(3), and (ii) unusual reverse regioselectivity in the reaction of $\mathbf{F_2}$. The results of our international collaborations, together with other recent results on this chemistry, will be presented at the symposium.

Keywords: allene; 2-bromo-1,3-diene; nucleophile; palladium; substitution





Masamichi Ogasawara Born in 1996. Univ. of Tokyo (Bachelor in 1989, Master in 1991, Ph.D. in 1994). Indiana Univ. (Postdoc, 1994-96 with Prof. Kenneth G. Caulton), Northwestern Univ. (Postdoc, 1996-97 with Prof. Tobin J. Marks), Kyoto Univ. (Assist. Prof. 1997-2002), Hokkaido Univ. (Assoc. Prof. 2002-2016), Tokushima Univ. (Professor 2016-present). [Field of research] Organometallic Chemistry, Asymmetric Synthesis.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-014)

Operando X-ray absorption spectroscopy development for catalytic ethanol reforming research

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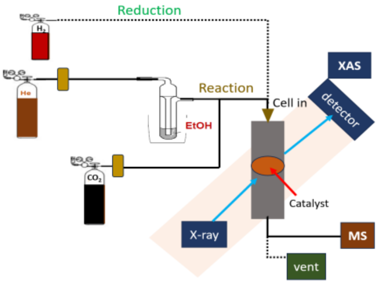
Carbon dioxide (CO_2), a major greenhouse gas emitted from fossil fuel combustion, significantly contributes to climate change. To mitigate CO_2 emissions, various strategies, including physical capture and chemical conversion into value-added products such as fuels, hydrocarbons, and carbonates, have been explored. The catalytic dry reforming of ethanol (DRE) presents a sustainable approach for syngas ($CO + H_2$) production by utilizing CO_2 as a carbon source and bioethanol as a renewable feedstock. This process highlights the need for innovative catalyst design and process integration to enhance industrial viability.

In this study, in situ/operando X-ray absorption spectroscopy (XAS) was employed to investigate the electronic and structural properties of M/LTL catalysts (M = Co, Cu, Ni) under reaction conditions. The combination of XAS with mass spectrometry (MS) enabled real-time monitoring of catalyst activity, selectivity, and stability for CO_2 reforming of ethanol. Our findings indicate that, after catalyst pretreatment at 300 °C, Cu metal species were predominant with no detectable Cu(I) phase, whereas Ni and Co oxides remained largely unreduced. Among the tested catalysts, Cu/LTL exhibited superior ethanol conversion and syngas selectivity, effectively initiating ethanol dry reforming at 550°C, where complete ethanol transformation was observed. This high performance is attributed to electron transfer from the reduced support to active metallic sites, facilitating C–C bond dissociation at the Cu interface. In contrast, Co/LTL and Ni/LTL catalysts demonstrated selectivity for side reactions at temperatures below 500°C. Notably, all metal catalysts-maintained stability throughout catalytic testing. These insights provide a fundamental understanding of catalytic behavior in ethanol dry reforming and guide the development of efficient catalysts for sustainable syngas production.

Keywords: ethanol; CO_2; operando XAS; syngas 4



Dr. Yingyot Poo-arporn is a Beamline Scientist at the Synchrotron Light Research Institute, specializing in synchrotron radiation, X-ray absorption spectroscopy, and catalytic reactions. He earned his Ph.D., M.Sc., and B.Sc. in Chemistry from Kasetsart University. His research on photocatalysis, electrochemical sensing, and green fuel production is published in leading journals like Materials Science in Semiconductor Processing and Sensors & Actuators: B. Chemical.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-015)

Characterisation of various materials using XAFS spectra at Photon Factory

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Institute of Materials Structure Science (IMSS) belongs to High Energy Accelerator Research Organization (KEK) located in Tsukuba, Japan. We operate two synchrotron rings, named Photon Factory (PF) and Photon Factory Advanced Ring (PF-AR). PF runs with the beam energy of 2.5 GeV, while PF-AR with 6.5 or 5.0 GeV provides higher energy regions. We have 6 x-ray absorption fine structure (XAFS) beamlines out of about 50 beamlines there. XAFS is one of the most widely used methods at synchrotrons and is applied to study various materials such as catalysts, batteries, magnetic materials, functional oxides, and environmental samples. XAFS spectra are usually divided into two characteristic regions: x-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS). XANES is the region of the spectrum from just below the absorption edge to ~50-70 eV above the edge and is used to clarify chemical/valence states. EXAFS includes the higher energy region above XANES and analysed to obtain local structures such as bond lengths and coordination numbers.

We would like to share a couple of XAFS studies performed at our facility. For example, Ce-doped CaF_2 is a laser material fabricated long before, but the dopant properties were unveiled. Our XAFS experiments revealed that Ce are doped in its Ce(III) state and substituted for the Ca site. We would touch a recent style utilisation of XAFS spectra, which are aided/driven by data, database and computers.

Keywords: synchrotron radiation; X-ray absorption spectroscopy; chemical state; local structure; bond length

Born in 1980. Graduated from the University of Tokyo. In 2008, Received PhD from the University of Tokyo, and appointed as Assistant Professor at Keio University. In 2010, became Associate Professor at IMSS, KEK. Also, appointed as Associate Professor at Ibaraki University from 2019. Research interest in synchrotron science, surface/interface science, low dimensional materials/ systems, and food science. A member of Executive Committee of International X-ray Absorption Society (IXAS) from Jul 2018, a member of International Union of Crystallography (IUCr) Commission on XAFS from Aug 2021, and a vice president of International Radiation Physics Society (IRPS) from Sep 2024.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-016)

Structural isomerization and molecular adsorption properties of ligand-protected metal clusters studied by XAFS

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Metal clusters, composed of less than ca. 100 atoms, are expected to show peculiar chemical properties that are essentially different from those of the corresponding bulk metals because of the unique geometric and quantized-electronic structures. Therefore, structural analysis with atomic precision and dynamic analysis of the structures and electronic states during the reaction are required. X-ray absorption fine structure (XAFS) analysis is a powerful tool to determine the local structure and electronic state of the specific elements under any condition such as solid, liquid, and gas phases. Our group applied the XAFS to the analysis of the geometric structures and vibrational properties of ligand-protected metal clusters, and to elucidation of the structural and electronic dynamics of the metal clusters during the reaction. In this talk, I will introduce two topics. One is the structural isomerization induced by the cluster packing between cationic $[MAu_8(PPh_3)_8]$ (M=Au, Pd, Pt, MAu8) and anionic polyoxometalates ($[Mo_6O_{19}]$ (Mo6), $[PMo_{12}O_{40}]$(PMo12)). The crown-motif PdAu8 and PtAu8 in the solution were isomerized to butterfly-motif structures by the association with Mo6 although it was predicted that the structural isomerization from crown-motif to butterfly-motif structure was suppressed in PdAu8 and PtAu8 by the higher activation energy and stiffer radial M–Au (M = Pd, Pt) than Au9. The core structures and bond stiffness in the core could be determined by XAFS. Second topic is the study on molecular adsorption behavior on Pt in $[PtAu_8(PPh_3)_8]$- $H[PMo_{12}O_{40}]$ (PtAu8-PMo12) solid. We successfully evaluated the adsorption speed of H_2 and CO on Pt in PtAu8-PMo12 solid by *in-situ* quick-scan XAFS with a time resolution of 0.1 s. We found that H_2 was adsorbed more rapidly (<0.5 s) on Pt than CO (~2.5 s) and showed reversible adsorption/desorption behavior on Pt atoms in PtAu8-PMo12 whereas CO was irreversibly adsorbed on Pt with structural isomerization.

Keywords: XAFS; metal cluster; isomerization; gas adsorption; structure

Seiji Yamazoe received his PhD degree in 2008 from Kyoto University. That same year, he transferred to the Department of Materials Chemistry, Ryukoku University as an Assistant Professor and in 2012 was appointed as an Assistant Professor in the Department of Chemistry, the University of Tokyo. In 2017, he was promoted to Professor at Tokyo Metropolitan University.

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-017)

Integrating *operando* X-ray absorption spectroscopy (XAS)-mass spectrometry (MS)-gas chromatography (GC) technique for characterization of cobalt-based catalysts in ethanol dehydrogenation and reverse water gas shift reaction

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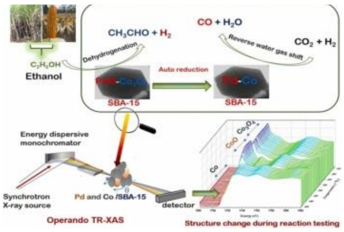
X-ray absorption spectroscopy (XAS) is an element-selective technique, a direct measure of the valence state. The consequence makes XAS, the technique particularly well-suited to the study of complex materials. *Ex situ* XAS only detects the catalyst state before or after the reaction, missing dynamic changes occurring under reaction conditions. *In situ* XAS provides insights into catalyst evolution under reaction-like real conditions but lacks direct measurement of catalytic performance. To bridge these gaps, we demonstrate in this work the *Operando* XAS-MS-GC technique by simultaneously monitoring catalyst structure (XAS) and reaction products (MS/GC), enabling a direct probing relationship of catalyst structure and catalytic activity under real reaction conditions. Herein, we applied *operando* time-resolved XAS (TR-XAS) to investigate an alternative reduction pathway of Pd-promoted Co_3O_4/SBA-15 under ethanol dehydrogenation and decomposition (ED). This technique could allow us to understand the insight nature of materials. Catalysts (xPd-10Co/SBA-15, x = 0.2, 0.5, 1.0 wt%) were synthesized via co-impregnation. The precursors were transformed to PdO and Co_3O_4 after calculation and to metallic form after reduction. The reducibility of Co_3O_4 to metallic Co in 1Pd-10Co/SBA-15 was 98.0%, whereas the metallic form was not produced in the absence of Pd. This catalyst achieved an 80% H_2 yield from ED at 500 °C. The ED-reduced 1Pd-10Co/SBA-15 was tested in the reverse water gas shift (RWGS) reaction using *operando* TR-XAS, achieving 97.8% CO selectivity—slightly higher than its H_2-reduced counterpart. Both reduction methods yielded comparable RWGS activity. These findings provide valuable insights into catalysts, both *operando* reduction via ED and RWGS reactions impacting catalytic performance, offering a foundation for optimizing bimetallic catalyst design.

Keywords: cobalt; palladium; ethanol dehydrogenation; reverse water gas shift; *operando* TR-XAS



Dr. Nattawut Osakoo (b. 1986) received a Ph. D. in chemistry in 2014 from Suranaree University of Technology (SUT). He is currently a researcher at SUT, focusing on value-added chemical synthesis from ethanol via non-oxidative dehydrogenation and CO_2 *hydrogenation, combined with operando XAS investigation. He co-authored 39 publications (h-index of 15, Scopus) and received several awards including an Outstanding Reviewer Award for Materials Research Express Journal in 2020 and an Outstanding Research Award in the physical science category from Synchrotron Light Research Institute, Thailand in 2023.*

Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-I-018)

Mechanistic insights into C-F bond activation and N-heterocycle functionalization by metal-ligand cooperative catalysts: Distinct bonding interactions

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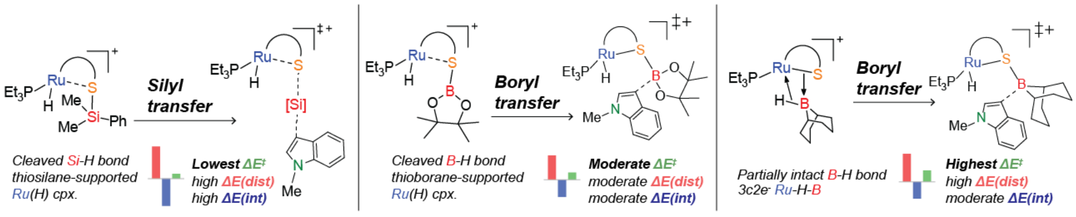
Density functional theory (DFT) calculations have provided insights into the mechanisms of C-F bond activation and N-heterocycle functionalization facilitated by metal-sulfur cooperative catalysts. Investigations into the hydrodefluorination of CF_3-substituted aniline derivatives, $CF_3(C_6H_4)NMe_2$, using the Ru-S complex $[(PEt_3)Ru(DmpS)]^+$ (DmpS = 2,6-dimesitylphenyl thiolate) with hydrosilane and hydroalane revealed distinct bond activation pathways. Si-H activation of $HSiMe_2Ph$ forms a Ru–H complex with a thiosilane ligand, requiring Si-S bond cleavage to generate an active silylium cation for fluoride abstraction. Conversely, Al-H activation of $HAliBu_2$ yields a Ru–H complex with the alumenium ($^{+}Al^{i}Bu_2$), stabilized by the donation from both σ(Ru-H) bond and the sulfur lone pair. The fluoride abstraction by the alumenium has a higher interaction and involves less structural change than that by the silylium. Additionally, the Ru-S complex also catalyzes C-H silylation and borylation of N-heterocycles, essential processes in synthesizing organic building blocks. Mechanistic studies on C-H silylation of 1-methylindole using hydrosilanes and C-H borylation using hydroboranes revealed four key steps: (i) Si–H/B–H activation, (ii) silyl/boryl transfer, (iii) proton abstraction, and (iv) H_2 elimination. Notably, Si-H/B-H activation formed distinct intermediates. Differences in bonding interactions influenced the energy barriers in the rate-determining silyl/boryl transfer steps, providing critical insights into catalyst design for C-H functionalization.

Keywords: metal-ligand cooperativity; N-heterocycle; silylation; borylation; C-F bond activation



Panida Surawatanawong, Texas A&M University at College Station, USA (Ph.D.), Max Planck Institute for Bioinorganic Chemistry, Germany (Postdoctoral Research Fellow), Mahidol University, Thailand (Associate Professor). Major Recognition/Awards: L'Oréal-UNESCO for Women in Science Award 2019, TRF-OHEC Scopus Young Researcher Award 2017, Young Scientist Award 2016. Research Interests: Computational Chemistry for Catalysis and Sustainability.

Catalytic Systems for Contemporary Challenges (S2-I-002)

Catalyst design for acceleration of unconventional electro-assisted molecular conversions: Beyond the thermodynamic equilibrium limit

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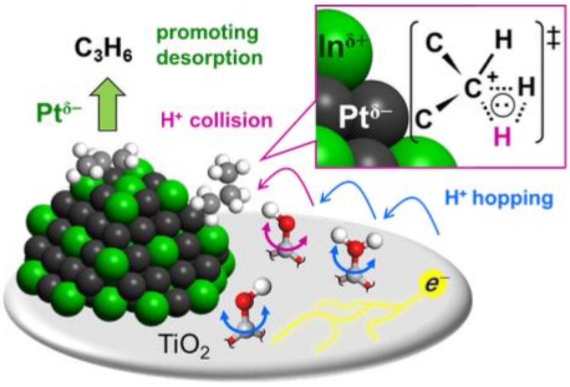
Many industrial chemical processes, where conversion rates are limited by chemical equilibrium, require high temperatures for the reaction to proceed, regardless of the performance of the catalyst, and must therefore be energy-intensive processes. Various approaches using electrochemical and photochemical energy have been attempted to break free from the constraints of such chemical equilibria.

Electrochemistry and photocatalysis aretypical examples, but these systems are notvery compatible from an engineering point ofview with large-scale industrial processesbased on gas-phase flow-type reactions due toproblems with gas diffusion in the electrolyteand light irradiation efficiency. In thispresentation, we introduce novel reactionsystems using "**electric field**" and "**plasma**" that can break the thermodynamicequilibrium limitations of endothermicreactions such as propane dehydrogenationand CO_2 reduction to CO, allowing asignificant reduction in the operatingtemperature. In addition, we show how to design functional catalysts that can accelerate such electro-assisted reactions and the importance of alloy materials for this purpose.

Keywords: electric field; surface protonics; plasma; propane dehydrogenation; CO_2 conversion



Dr. Shinya Furukawa received his Ph.D. from Kyoto University in Mar. 2012. He joined the Tokyo Institute of Technology as an assistant professor in Apr. 2012. He moved to Hokkaido University as an associate professor in June 2016 and was promoted to full professor at the University of Osaka in May 2023. He specializes in heterogeneous catalysis using advanced multimetallic materials such as high-entropy intermetallics. He also works on the development of conventional and unconventional catalytic systems using electricity for innovative molecular conversions. The target reactions are typically hydrocarbon refining, CO_2 utilization, and hydrogen production.

Catalytic Systems for Contemporary Challenges (S2-I-004)

Miniaturized wireless electrochemical flow reactor for complex tasks

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Serena Arnaboldi[1,*]
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Enantiopure asymmetric synthesis is crucial for the pharmaceutical industry, but traditional electrocatalysis suffers from mass transport limitations and byproduct formation. Herein we present a novel approach leveraging the synergy between bipolar electrochemistry and inherently chiral conjugated polymers to develop wireless flow reactors for asymmetric electrosynthesis. [*Chem* **2023**, *10*, 1–15; *Anal. Chem.* **2024**, *96*, 4901–4908] Tubular polypyrrole (Ppy) devices, functionalized with enantiopure oligomers, act as these wireless chiral reactors. The Ppy outer shell functions as a wireless micro-pump, driven by an external electric field, ensuring efficient mass transport of the prochiral substrate. Simultaneously, the inner shell provides the chiral environment for enantioselective reactions. We demonstrate the enantioselective reduction of acetophenone to 1-phenylethanol within this system. Fine-tuning the applied electric field allows for the production of 1-phenylethanol with high enantiomeric excess (>90%) and conversion efficiency (>90%). This sustainable and wireless method offers a green alternative for the production of enantiopure compounds, holding significant promise for applications in pharmaceuticals, chemistry, and materials science.

Keywords: asymmetric electrosynthesis; bipolar electrochemistry; chiral conjugated polymers; wireless microreactors; enantioselective reduction

Serena Arnaboldi is currently an Associate Professor in Analytical Chemistry at the Department of Chemistry, University of Milan (Italy). After receiving her PhD in 2014 from the University of Milan, she moved to Bordeaux to work with Alexander Kuhn. In 2021, she was awarded an ERC Starting Grant for a project focused on the transmission of chirality across length scales. Her primary research interest lies in chiral electrochemistry, including areas such as enantioselective electroanalysis, enantioselective electrosynthesis, chiral bipolar electrochemistry, and self-propelled electrochemical actuators. Her work has implications for the development of new chiral separation techniques and the synthesis of enantiomerically pure compounds.

Catalytic Systems for Contemporary Challenges (S2-I-018)

Nickel phyllosilicate catalyst derived from bagasse fly ash for H_2 production via dry reforming of methane

Nataphon Meeboonanake, Wasawat Kraithong, Anan Jiratanachotikul, Aniwat Pengsawang, Sanchai Kuboon*
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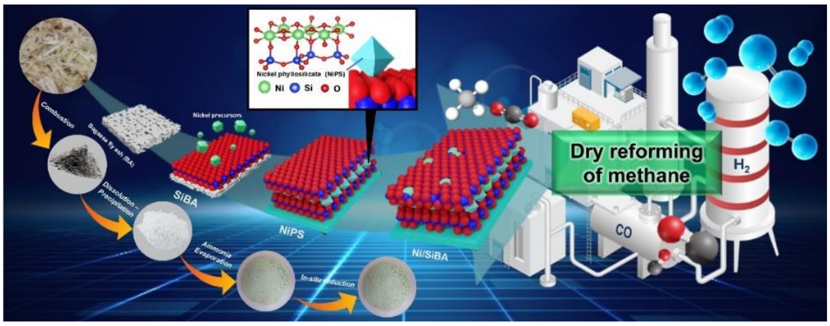
In this work, high surface area non-synthetic silica (>500 m^2/g) was extracted from bagasse fly ash (SiBA), an industrial biomass waste, and employed as a support for nickel-based catalysts (Ni/SiBA) with Ni loading ranging from 1 to 15 wt%. The catalysts were synthesized via a simple ammonia evaporation (AE) method and characterized using XRD, N_2 physisorption, H_2-TPR, H_2-TPD, and ICP-OES. Catalytic performance was evaluated for dry reforming methane (DRM) at 750°C under a 1:1 molar CH_4 and CO_2 reactant ratio. The catalyst with 10 wt% Ni loading exhibited the highest activity, achieving CH_4 and CO_2 conversion of 93% and 98%, respectively, and an H_2/CO ratio of 1.15 after 10 h on the stream. Enhanced performance was attributed to the formation of nickel phyllosilicate and well-dispersed Ni nanoparticles. Stability testing over 35h confirmed sustained activity, with CH_4 conversion above 80% and near-complete CO_2 conversion. Post-reaction analyses (TEM, TPO, Raman, XRD, TGA) indicated minimal carbon deposition and structural stability. These findings demonstrate the potential of Ni/SiBA as a cost-effective and durable catalyst for syngas and hydrogen production via DRM while supporting sustainable waste valorization.

Keywords: dry reforming of methane; bagasse fly ash; nikel catalyst; silica support; syngas production



Sanchai Kuboon obtained his Ph.D. from Michigan Technological University in Materials Science and Engineering. He is currently a senior researcher at Catalyst Research Team, Nanocatalysis Adsorption and Simulation Research Group at the National Nanotechnology Center (NANOTEC), NSTDA, Thailand. His research is mainly focused on biomass conversion and utilization using biorefinery and torrefaction approaches. He is also actively working on CO_2 conversion and utilization via thermochemical processes.

Catalytic Systems for Contemporary Challenges (S2-I-020)

Towards ultrahigh osmotic energy harvesting by MOF and COF based ionic diode membranes

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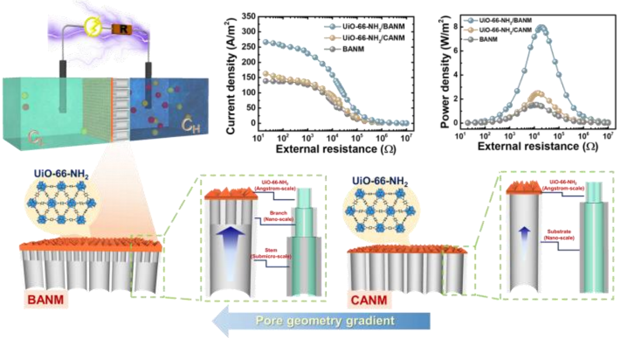
The chemical energy stored between seawater and river water, the so-called osmotic energy (or blue energy), can be harvested by an ion-selective membrane. However, previously reported membranes suffer from insufficient ion selectivity and inferior transmembrane ionic flux (low conductance), thus impeding practical application. For example, the output osmotic power density reported by most of existing ion selective membranes is typically below the commercial benchmark of 5 W/m^2. Taking the inspiration from electrocytes in electric eel, which consist of a large number of sub-nanoscale rectified ion channels that allow unidirectional ion transport with amplified flux, we engineered two types of sub-2 nm-scale covalent-organic framework (COF) and metal-organic framework (MOF) based ionic diode membranes for osmotic energy harvesting. We show that the two COF and MOF-based heterogeneous membranes can rectify ionic current even in high salt concentration. We then probe application of these mem-branes in harvesting energy from salinity gradients. Notably, in addition to ultrahigh ion selectivity, these sub-2 nm-scale ionic diode membranes can achieve an unprecedented power density, higher than the commercial bench-mark bandgap and outperforms all the state-of-the-art ion selective membranes. Our works would open up new avenues of using pinhole-free COF and MOF membranes towards next-generation highly selective and ultra-high-performance sustainable energy harvesting.

Keywords: ion transport; ion selective membrane; ion current rectification; metal-organic framework; covalent-organic framework



Angew. Chem. Int. Ed. 2024, 63, e202408375

Dr. Li-Hsien Yeh is a distinguished professor in the Department of Chemical Engineering at the National Taiwan University of Science and Technology. He received his Ph.D. in Chemical Engineering from National Taiwan University in 2007. He was awarded the SCEJ Award for Outstanding Asian Researcher and Engineer from the Society of Chemical Engineers (SCEJ), Japan (2020), and the Outstanding Research Award from the National Science and Technology Council, Taiwan (2023). He is currently an Editor of Chemical Engineering Journal. His current research interests include microfluidics and nanofluidics, MOF/COF/2D materials/hydrogel, ion transport membranes, and nanofluidic energy conversion.

Catalytic Systems for Contemporary Challenges (S2-I-024)

Preparation of Janus particles by bipolar electrochemistry at the water-organic interface

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Janus particles have a wide range of applications in diverse fields due to the possibility to tailor and combine different functionalities on a single particle. However, most of the current techniques for the synthesis of Janus particles are still suffering from limited control of the generated asymmetry. Therefore, achieving the synthesis of bi-functionalized Janus particles with a completely tunable modification ratio between two components is still extremely challenging. In this context, bipolar electrochemistry offers unique advantages to achieve controlled asymmetry in terms of the precise spatial distribution of electrochemical reactions at the two polarized extremities of a bipolar electrode. We propose herein a new approach to synthesize Janus particles at the water/organic (w/o) interface by bipolar electrochemistry. Janus particles with varying degrees of amphiphilicity are first prepared by bipolar electrochemistry, and are then positioned at the w/o interface. Subsequently, highly controlled bi-functionalization is achieved by carrying out different electrochemical reactions on their two sides. The ability to selectively modify the hydrophilic and hydrophobic regions allows for the generation of Janus particles with tailored properties at each face. This approach can be adapted for the synthesis of asymmetric particles with different dimensions, having various compositions and functionalities, thus opening up potential applications, ranging from catalysis to the delivery of active compounds.

Keywords: Janus particles; bipolar electrochemistry; water-organic interface

Dr. Lin Zhang is a professor at the Engineering Research Center for Nanomaterials, Henan University in China. Her academic career begins with a Bachelor's degree in Chemistry from Henan University, followed by a joint Master's degree in Advanced Functional Materials through the Erasmus Mundus program at the Universities of Bordeaux (France) and Augsburg (Germany) from 2011 to 2013. She obtained her Ph.D. in Chemistry from the University of Lorraine, France (2013-2016), and conducted postdoctoral research at the University of Bordeaux (2017-2018). Her current researches involve bipolar electrochemistry, electroenzymatic synthesis, electroanalysis, and the electrochemical synthesis of nanoparticles.

Catalytic Systems for Contemporary Challenges (S2-I-025)

Understanding the role of copper-based materials in electrochemical applications

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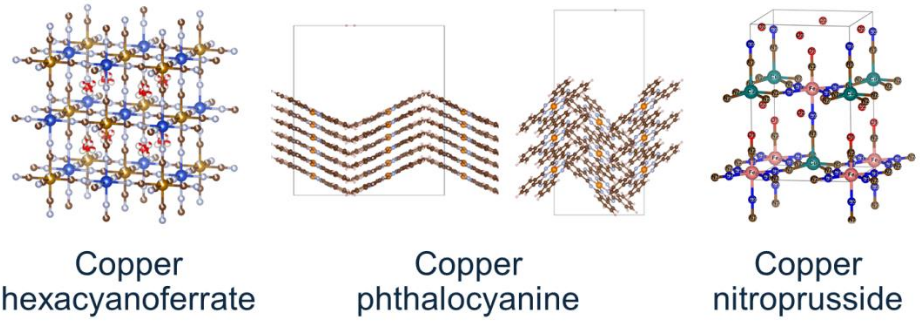
Copper-based materials have emerged as highly versatile and efficient platforms for a wide range of applications, from energy conversion to environmental monitoring. This talk will explore the electrochemical behavior of copper compounds such as copper phthalocyanine, copper nitroprusside, copper hexacyanoferrate, and copper oxides, with a focus on charge transfer properties and surface interactions. By integrating electrochemical techniques, computational studies, and structural characterization, we provide insights into mass transport and redox mechanisms, contributing to the development of more efficient and selective platforms for sensing, electrocatalysis, and other electrochemical technologies.

Keywords: electrochemistry; copper centers; charge transfer; redox mechanisms



Associate Professor Dr. Kamonwad Ngamchuea obtained a Master of Chemistry (First Class Honours) in 2015 and a D.Phil. in Physical and Theoretical Chemistry in 2018, both from the University of Oxford, UK. She has been at the School of Chemistry, Suranaree University of Technology since 2018. Dr. Ngamchuea has been recognized with awards such as the Educational Award for Excellence (2017), the RSC Ronald Belcher Award (2018), and the Young Scientist Award (2022). Her research focuses on electrochemistry and electroanalysis.

Catalytic Systems for Contemporary Challenges (S2-I-026)

Rational design of zeolite-based catalysts for industrially relevant chemical processes

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Light olefins, especially propylene, are key building blocks in the petrochemical industry, mainly produced via steam cracking of hydrocarbons or fluid catalytic cracking (FCC) of heavy feedstocks such as vacuum gas oil (VGO). The latter process presents the advantages of its ability to handle heavy oil fractions and to selectively adjust the product distributions. One of the most cost effective and efficient routes to enhance light olefins yield is the addition of catalyst additives to USY-based FCC catalysts. The medium pore zeolite ZSM-5 is one of the most studied FCC additives, producing predominantly propene and butenes but also light alkanes by undesired bimolecular hydrogen transfer reactions. Thus, the design of new additives with higher selectivity to LPG olefins is of high interest.

Herein, we have designed an efficient additive based on a composite material derived from ZSM-5 and layered double hydroxides (Z5-LDH). The increase in LPG olefin production is attributed to the lower Brønsted acid sites and acid strength in Z5-LDH, which minimizes secondary reactions such as hydrogen transfer. Moreover, the basic metal oxide generated from the LDH material suppresses the re-adsorption of produced LPG olefins, reducing their conversion and increasing their final yield. This additive has shown benefits not only in VGO cracking but also in the conversion of other heavier feedstock such as ATM residue.

Keywords: zeolite/LDH; FCC additive; catalytic cracking; heavy oils; propylene

Cristina Martínez, born in Enschede (The Netherlands) in 1967, is a Tenured Researcher of the Spanish National Research Council (CSIC) at the Institute of Chemical Technology, UPV-CSIC, in Valencia, Spain. She received her B.S. degree in Chemistry at University of Valencia in 1991 and completed her PhD in Chemistry at the Polytechnic University of Valencia in 1996. Her research is focused on the application of optimized heterogeneous catalysts, mainly zeolite based, to industrially relevant processes within the refining and petrochemical areas. She has 70 publications in international peer-reviewed journals and 19 patent applications.

Catalytic Systems for Contemporary Challenges (S2-I-027)

Advances in tailored functional nanomaterials on microfluidic paper-based devices for optical sensing innovations

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[2]Department of Chemistry and Center of Excellence for Innovation in Chemistry, Ubon Ratchathani University, Ubon Ratchathani 34190, Thailand.
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My research in analytical chemistry at Ubon Ratchathani University, Thailand, focuses on developing sustainable, low-cost technologies aligned with Green Chemistry principles. Utilizing microfluidic paper-based analytical devices (µPADs) integrated with various functional nanomaterials—including Silver Nanoparticles (AgNPs), Silver phosphate nanocomposite (Ag_3PO_4/Ag), Nitrogen-doped carbon dots/Ni-MnFe-layered double hydroxides (N-CDs/Ni-MnFe-LDHs), Gold nanoparticles (AuNPs), Vanadium-doped porous cobalt oxide (v-porous Co_3O_4), and nitrogen-doped carbon dots (N-CDs). I design eco-friendly sensors for environmental monitoring, food safety, and diagnostics. These innovations minimize harmful chemical use and waste while delivering high sensitivity and selectivity.

For example, N-CDs are synthesized via a nontoxic hydrothermal method and applied as peroxidase mimics and fluorescent probes. In one study, N-CDs enabled colorimetric detection of total cholesterol in whole blood using 3D-µPADs, requiring no sample preparation and providing results in under 10 minutes. Another application utilized N-CDs in a fluorescence-based portable device for detecting formalin in food. The fluorescence "off-on" mechanism ensured rapid, sensitive analysis comparable to standard methods. Further, N-CDs served as fluorometric probes for detecting lead and cadmium in environmental water and herbal samples, achieving low detection limits with minimal reagent consumption. Additionally, a paper-based test kit for cyanide detection showcased high sensitivity via an "off-on" fluorescence mechanism.

These µPADs are low-cost, easy to fabricate, scalable, and ideal for field-based monitoring, reducing environmental impact and supporting pollution prevention. My work demonstrates the potential for these devices to advance chemical and biochemical sensing for broader applications, including real-time environmental, food, and diagnostic monitoring.

Keywords: microfluidic paper-based analytical devices (µPADs); functional nanomaterials; green chemistry principles; environmental and food monitoring; point-of-care testing

Purim Jarujamrus (born August 12, 1984) is an Associate Professor at the Department of Chemistry, Ubon Ratchathani University, Thailand. He received his Ph.D. in Analytical Chemistry from Mahidol University, Thailand, in 2012. Since 2024, he has served as the National Representative (NR) of Thailand in the Analytical Chemistry Division of IUPAC. His research focuses on the development of functional nanomaterials for fiber-based microfluidic analytical devices for innovative chemical and biosensing applications. To date, he has published approximately 90 articles in peer-reviewed journals.

Catalytic Systems for Contemporary Challenges (S2-I-030)

Biopolymer-stabilized gold nanoparticles for the organic transformation catalyst

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Gold nanoparticles (AuNPs) stabilized by biomacropolymers such as cellulose, chitin, and chitosan have attracted considerable attention in the context of sustainable development, owing to the abundance and renewability of these biopolymers. Moreover, the inherent structural and functional diversity among these macromolecules impart distinct catalytic properties to the resulting nanomaterials. In this presentation, I will discuss the size-controlled synthesis of AuNPs stabilized by chitosan [*J. Mol. Catal. A: Chemical* **2011**, *341*, 1.; *J. Nanopart. Res.* **2023**, *25*, 50] or citric acid-modified fibrillated cellulose [*ACS Omega* **2020**, *5*, 33206.] and highlight their unique catalytic performance in various organic transformation reactions. [*Chem. Asian J.* **2012**, *7*, 55; *Sci. Rep.* **2022**, *12*, 20602; *Nanoscale* **2024**, *16*, 12474; *Synlett* **2024**, *35*, 2417]

Keywords: gold nanoparticles; biomacropolymers; organic transformation

Hidehiro Sakurai received his Ph.D. degree from U. Tokyo in 1994. After being Assistant Professor in Tokyo (1994–1996, 1998–2000), JSPS Postdoctoral fellow at U. Wisconsin (1996–1998), and an Associate Professor in Osaka U. (2000-2004), he moved to the Institute for Molecular Science (IMS). In 2014, he returned to U. Osaka. Professor Sakurai has studied various topics in physical organic chemistry, and his current research interests include the science of buckybowls, and nanometal catalysts.

Catalytic Systems for Contemporary Challenges (S2-I-031)

Gallium based catalysts for selective chemical synthesis

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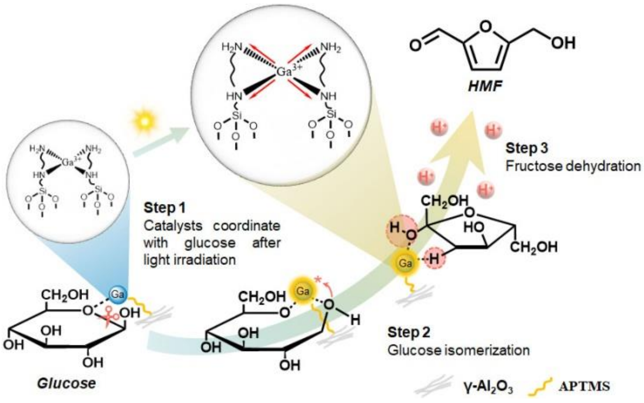
Extremely limited research exploring the photocatalytic potential of main group metals, such as aluminum, gallium, and tin, has been undertaken due to their weak light harvesting properties. This study reports the efficient transformation of sugars to 5-hydroxymethylfurfural (HMF) with high yield employing an original heterogenous photocatalyst comprising a gallium(III) complex immobilized on an alumina support. Under visible light irradiation, the turnover number (TON) of the heterogeneous gallium(III) photocatalyst was as high as 1500, which was ca. two orders of magnitude higher than the TON of the homogeneous gallium(III) system. It is proposed that photoirradiation significantly enhances the Lewis acidity of the catalyst by forming a semi-coordination state between gallium(III) and N-donor ligands, enabling the increased interaction of reactant sugar molecules with gallium(III) active sites. Consistent with this, the photoresponsive coordination of the gallium(III) complex and the abstraction of the hydroxy group by the metal under irradiation with visible light is observed by NMR spectroscopy for the first time. These findings demonstrate that efficient photocatalysts derived from the main group elements can facilitate biomass conversion using visible light.

Keywords: main group elements; biomass conversion; ammonia; liquid metal



Dr. Sarina (born in 1984) is an Associate Professor and ARC Future Fellow in the School of Chemical and Biomolecular Engineering, the University of Sydney. She received her PhD in 2013 from Queensland University of Technology (Australia) and was awarded the Alexander von Humboldt Fellowship (2014) and ARC DECRA Fellowship (2019). Her research is focusing on metal nanoparticle based plasmonic catalysis for solar driven chemical synthesis. She published over 60 articles in high-ranking journals and received many awards like the "2021 Energy and Fuels Rising Star" and now serving as the Associate Editor of Materials Today Sustainability and Cleaner Chemical Engineering.

Catalytic Systems for Contemporary Challenges (S2-I-032)

Histidine stabilization for supported metal nanoparticles: A simple trick for a big problem in thermal catalysis

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[1]*Department of Chemical and Process Engineering, The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Christchurch, New Zealand*
[2]*Department of Chemistry, The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Otago, Dunedin, New Zealand*
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Catalyst durability has emerged as a central issue in catalysis, primarily due to the sintering or agglomeration of metal nanoparticles, which leads to deactivation. We have developed a method that involves the addition of histidine, an amino acid known for its ability to bind with metals, to a palladium salt solution during its dissolution in water, with fumed silica serving as the support material. The imidazole functional group in histidine facilitates the uniform distribution of Pd particles and prevents their agglomeration during propylene hydrogenation. Our TEM and STEM images vividly demonstrate how histidine can disperse large Pd clusters into finer nanoscale particles, thereby enhancing the active surface area of the catalyst and its performance.

Our results indicate that the histidine not only prevents the sintering of Pd particles but also, upon decomposition, leaves behind a catalyst with significantly improved Pd nanoparticles dispersion and catalytic performance. The Pd/SiO_2 catalysts modified with histidine demonstrate superior stability during propylene hydrogenation up to 200 h, underscoring the practical implications of our findings for the design of robust and durable catalytic materials in industrial applications.

Keywords: supported metal catalyst; sintering; stability; activity

Professor Alex Yip (b. 1979) earned his BE (Hon) in Chemical Engineering from UNSW Australia in 2003 and his Ph.D. in heterogeneous catalysis from HKUST in 2009. After a postdoctoral fellowship at UC Berkeley, he joined the University of Canterbury in 2011, where he leads the Laboratory for Energy and Environmental Catalysis. His research focuses on zeolites and heterogeneous catalysts for sustainable energy, carbon neutrality, hydrogen energy, CO_2 utilization, biomass conversion, and gas separation. He has published over 120 journal articles and serves as an assessor for major research funds across Australia, New Zealand, Hong Kong, the USA, and Europe.

Advanced Coordination Materials and Catalysis for Environment (S3-I-003)

Development of supramolecular frameworks of metal-organic carboxylates

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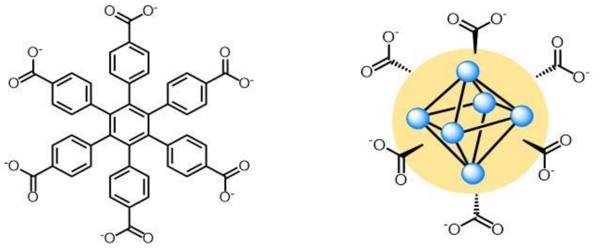
**E-mail: nobuto@chem.sci.osaka-u.ac.jp*

Organic carboxylates are fundamental building units for constructing coordination and hydrogen-bonded frameworks in supramolecular chemistry. Recently, discrete metal complexes with non-coordinating carboxy moieties (Metal-Organic Carboxylates; MOCs) have attracted increasing attention as alternatives to organic carboxylates because of their simple synthetic procedures and structural diversity, as well as the functionality due to transition metal centers. [*Coord. Chem. Rev.* **2023**, *474*, 214850] Inspired by the historically important Cu_{14} cluster with d-penicillamine, which is the first MOC, we have developed a variety of metallosupramolecular aggregates based on MOCs. In my talk, I will describe our recent achievements about the migration and condensation reaction of aqua metal species in the supramolecular frameworks. [*Angew. Chem. Int. Ed.* **2020**, *59*, 18048–18053; *Inorg. Chem.* **2024**, *63*, 6239–6247]



Organic Carboxylates

Metal-Organic Carboxylates (MOCs)

Keywords: metal-organic carboxylates; metalloligands; ionic conductor; cluster synthesis

Nobuto Yoshinari (b. 1982) is a professor at The University of Osaka; he received a B.Sc. degree in 2005, M.Sc. degree in 2007, and Ph.D. degree in 2010 from Osaka University (Japan). He started his academic career at Osaka University as an assistant professor in 2010 and was promoted to senior lecturer in 2016, associate professor in 2019, and professor in 2024. His research interests are focused on the rational creation of supramolecular assemblages of multinuclear metal clusters and the development of their solid-state functionalities

Advanced Coordination Materials and Catalysis for Environment (S3-I-004)

Single-ion conducting borate network polymer electrolytes for lithium metal battery applications

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Although it is possible to readily estimate the theoretical energy densities of battery chemistries, the molecular processes that hinder practical performance are still unknown. Especially, the charging and discharging rates have become a major limiting factor in energy storage applications. Several solid electrolytes with exceptional ionic conductivity have been discovered, but all-solid-state batteries with high energy density have been only realized at limited rates (close to equilibrium), indicating that the minimization of overpotential requires to be considered to improve the rate performance other than the ionic transport. As single-ion polymer electrolytes, in which only selective cations are mobile across polymer electrolytes, facilitate minimizing not only the concentration gradient but also the overpotentials in the cells, such electrolytes pose great potential for overcoming these problems. However, single-ion polymer electrolytes have suffered from low ionic conductivity ($<10^{-5}$ S cm^{-1} at ambient temperature) which is at least two orders of magnitude smaller than that of liquid electrolytes. In this talk, I will present our ongoing efforts to develop a new class of single-ion conducting polymer electrolytes using an interpenetrated network polymer with weakly coordinating anion nodes, with a wide electrochemical stability window, a high room temperature conductivity of up to 1.5×10^{-4} S cm^{-1}, and exceptional selectivity for Li-ion conduction ($t_{Li+} = 0.95$). Significantly, lithium metal battery prototypes containing these electrolytes are shown to outperform a conventional battery featuring a polymer electrolyte.

Keywords: single-ion conducting network polymer electrolytes; porous aromatic frameworks; lithium metal battery; polymer electrolyte

Dong-Myeong Shin is an Assistant Professor of Mechanical Engineering at the University of Hong Kong. He obtained a Ph.D. in nanomaterials (2016) from Pusan National University under the supervision of Profs. Yoon Hwae Hwang and Hyung Kook Kim. In 2017, he moved to the University of California, Berkeley as a postdoctoral scholar with Prof. Jeffrey R. Long. In 2019, he assume his current position where his group has devoted to developing self-powered nanoelectronics, with an emphasis on important components such as energy harvesting/storage devices.

Advanced Coordination Materials and Catalysis for Environment (S3-I-005)

Direct conversion of *n*-alkanes to alkylidynes on diruthenium complexes at ambient temperature

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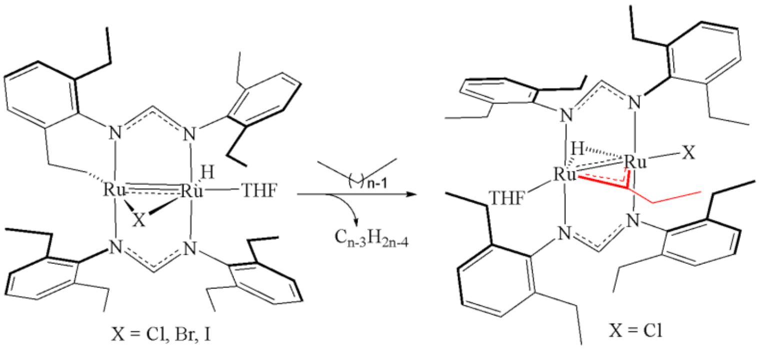
Cracking of light alkanes holds significant importance due to its focus on producing light olefins in a more energy-efficient and environmentally sustainable manner compared to conventional thermal cracking methods. Modern alkane cracking typically employs zeolites as catalysts, which are selected to maximize the yield of hydrocarbons with 5 to 10 carbon atoms–an ideal range for gasoline production. Furthermore, alkanes can undergo hydrogenolysis on metal catalyst surfaces, producing smaller alkanes under high hydrogen pressures and elevated temperatures, where alkylidyne intermediates play a key role. In this study, we report the cleavage of light alkanes (C_nH_{2n+2}) at ambient temperature using homogeneous mixed-valent diruthenium amidinate complexes. These reactions yield propylidyne complexes and lighter alkanes through a process involving the cleavage of two C−H bonds and one C−C bond, as well as the formation of a new C−H bond, resulting in the extrusion of lighter alkanes ($C_{n-3}H_{2n-4}$). The reaction mechanism has been elucidated through computational studies. Our findings highlight that low-coordinate, low-valent dinuclear ruthenium provides a distinctive platform for the activation of n-alkanes. This approach may pave the way for the development of novel catalysts designed to utilize alkanes more effectively in chemical synthesis.

Keywords: alkanes; cracking; ruthenium; C–H and C–C bond cleavage; alkylidyne



Yi-Chou Tsai, born in 1969, earned his Ph.D. from MIT in 2001 and subsequently completed postdoctoral training at Caltech (2001–2003). He is currently a professor at National Tsing Hua University, Taiwan. His research primarily focuses on the study of low-coordinate and low-valent dinuclear transition metal and main group metal complexes. He has received the Outstanding Research Awards from the National Science and Technology Council, Taiwan, in both 2014 and 2019.

Reactions of HMF, FDCA, and BHMF

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Integrated biorefineries have been receiving more attention to increase the demand responses in bio-green-circular economy for solving the environmental global issues leading to the sustainable development. 2,5-hydroxymethyl furfural (HMF), 2,5-furandicarboxylic acid (FDCA) and 2,5-bis(hydroxymethyl)furan (BHMF) are selected as chemical platforms to be investigated for this report. For the HMF chemical platform, metal-oxide catalysts will be reported for the oxidation of HMF to FDCA. HMF is an unstable molecule, and it is transformed to humin in an acidic solution or a high concentrated condition. The stabilization of HMF by the structure modification of HMF or the addition of other metal ions will be reported. For the BHMF platform, the Diels-Alder cycloaddition of BHMF and *N*-phenylmaleimide derivatives under optimal reaction conditions was investigated. Firstly, HMF was reduced to BHMF in the presence of $NaBH_4$ and then the Diels-Alder reaction of BHMF and *N*-phenylmaleimide derivatives was investigated to produce Diels-Alder adducts.

Keywords: HMF; FDCA; BHMF

Ekasith Somsook (b. 1972) received his Ph.D. in Chemistry from the University of Wisconsin-Madison. He is currently an Associate Professor at the Department of Chemistry, Faculty of Science, Mahidol University. His research focuses on catalysis for sustainability, particularly nanocatalysis, plastic recycling, and biorefinery.

Advanced Coordination Materials and Catalysis for Environment (S3-I-009)

Silsesquioxanes-based functional materials for sustainable development

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With the rapid development of industry, resources shortage and environment pollution are emerging. Therefore, it is emergent to find innovative materials to resolve these problems and meet the requirements of sustainable development. Cage-like silsesquioxanes have a rigid inorganic skeleton and organic groups at their peripheries forming organic–inorganic hybrid structures with light weight, good hydrophobicity, and ease of modification. Thus they can be considered to be ideal building components to prepare some target hybrid materials with specific functions, for example, catalysis, adsorption and separation, sensing and self-cleaning, etc. [*Progress in Polymer Science*, **2021**, *119*, 101419; *Adv. Funct. Mater.* **2023**, *22*, 2214875] Recently, we have designed and prepared some silsesquioxanes-based porous polymers, superhydrophobic coatings and aerogels *etc.*, which are successfully used as adsorbents, photocatalysts, sensors for environment remediation [*Surface and Coatings Technology* **2023**, *457*, 129285; *Chemical Engineering Journal* **2023**,*462*,142323]. We believe that more silsesquioxanes-based functional materials will be created and their application will be further expanded.

Keywords: silsesquioxane; function; hybrid fluorescence; photocatalyst

Hongzhi Liu was born in 1972 and obtained his PhD from Shanghai Jiao Tong University in 2005. He did his postdoctoral research at Gunma University, Japan from 2006 to 2009 and Vienna University of Technology from 2009 to 2011, funded by "Lise Meitner" Scholarship. In 2011 he joined Shandong University, China as a full professor. His current interest focus on functional silsesquioxane monomer synthesis and hybrid materials based on silsesquioxanes.

Advanced Coordination Materials and Catalysis for Environment (S3-I-010)

Silsesquioxane materials: Application to catalysis and to nanomedical fields

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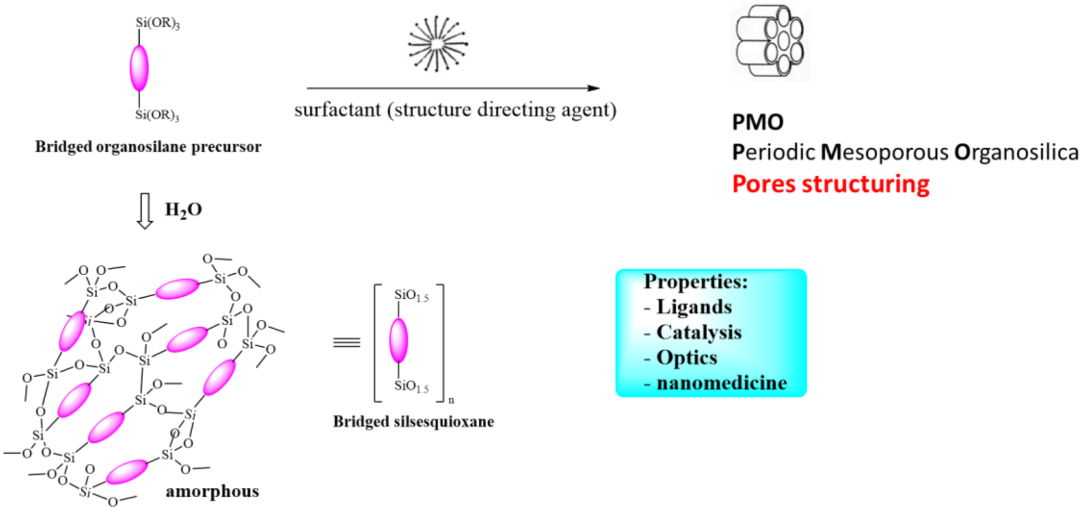
Organic-inorganic silica-based materials can be synthesized from bridged organosilane precursors. These hybrids can be prepared in several types and structures, known as bridged silsesquioxanes (**BS**) and Periodic Mesoporous Organosilicas (**PMO**). While the former **BS** is described as 'amorphous' materials, **PMO** can be obtained as nanoparticles with structured mesoporous pores called **nano-PMO** and Hollow Mesoporous Organosilicas (**HMON**). In this presentation, I will firstly give an example of a **BS** hybrid and demonstrate its application as efficient and recoverable/reusable catalyst. The syntheses of nano-PMO with structured and uniform-size pores will then be given and used in nanomedical application and finally preliminary results of sized-controlled HMON will be presented

Keywords: bridged silsesquioxane; periodic mesoporous organosilicas; catalysis; nanomedicine



Michel Wong Chi Man is a CNRS researcher. He received his Ph.D. in Chemistry from the University of Montpellier (France) and then completed a postdoctoral research as a Humboldt (AvH) fellow at the University of Heidelberg (Germany). He is an expert in organosilicon and hybrid silica chemistry, and his research interests focus on the functionalization of bridged silsesquioxanes for supported catalysis and stimuli-responsive hybrid silica nanoparticles, with applications in nanomedicine. He is a Board Member of several international meetings on silicon and sol-gel fields, ISOS and ISGC, and a fellow of the International Sol-Gel Society.

AI in Drug Discovery Research (S5-I-001)

Deep learning for identifying bioactive compounds and predicting drug synergy

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King Mongkut's University of Technology Thonburi
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The complex nature of biological systems and the vast chemical space of potential therapeutics require innovative approaches to drug discovery. This presentation discusses the use of deep learning and computational modeling to discover novel therapeutics. In the first project, we developed deep-learning models to identify potentially bioactive compounds derived from mushrooms. Integrating these predictions with molecular docking studies, we identified promising candidate inhibitors exhibiting favorable binding profiles for mTOR and acetylcholinesterase, targets relevant to cancer and Alzheimer's disease, respectively. In the second project, we addressed the challenge of predicting synergistic drug combinations in breast cancer. We created a deep neural network that predicts synergy based on the inhibitory activities of drug pairs against key cancer proteins. Although the model achieves only moderate predictive performance, its key advantage lies in its ability to interpret the protein-level mechanisms that drive synergistic effects. These projects demonstrate the potential of deep learning and computational modeling to accelerate the discovery and optimization of therapeutics across various disease areas.

Keywords: Alzheimer's disease; cancer; deep learning; drug synergy; molecular docking

Teeraphan Laomettachit, born in 1983, earned his B.Sc. in Biology from Chulalongkorn University and his Ph.D. in Genetics, Bioinformatics, and Computational Biology from Virginia Tech. He is currently an Associate Professor of Systems Biology in the Bioinformatics and Systems Biology Program, School of Bioresources and Technology, King Mongkut's University of Technology Thonburi. His research focuses on integrative approaches—including mathematical modeling, machine learning, and bioinformatics analysis—to understand the complexity of diseases and develop effective interventions.

AI in Drug Discovery Research (S5-I-002)

MANORAA.ai as a co-scientist for drug discovery

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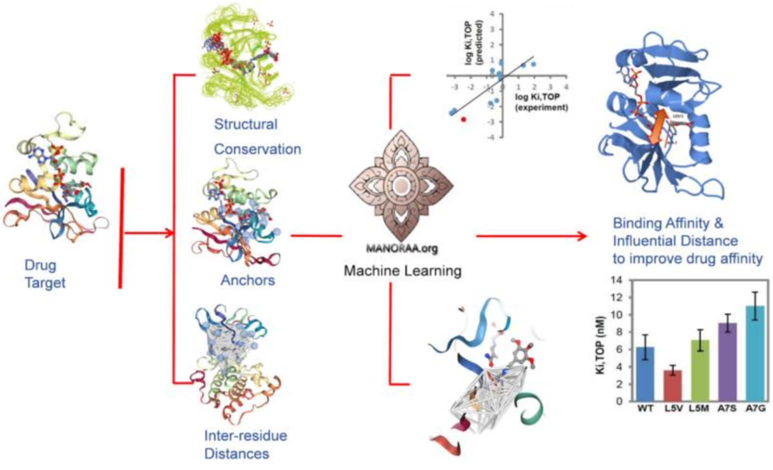
Drug design demands the analysis of extensive chemical and biophysical data, and requires integration from multiple scientific disciplines. This presentation explores an innovative AI-powered workflow where bioinformatics connects protein crystallographic data with biological functions and biochemical pathways. By applying data-driven models to protein-ligand binding interaction and active site boundary, I will showcase how MANORAA refines molecular design strategies. This methodology advances rational drug design by deciphering the intricate three-dimensional molecular puzzles of protein-ligand interactions and enhancing our understanding of biomolecular structures through influential distance equations and frequently occurring molecular patterns. With experimental validation from X-ray crystallography and kinetics data, this machine learning framework could streamline the drug discovery process—reducing costs, improving efficiency, and accelerating the development of new therapeutics. When properly implemented, it has the potential to revolutionize pharmaceutical innovation and protein engineering (https://manoraa.org).

Keywords: protein, biomolecules, drug design, platform, co-scientist



Dr. Duangrudee Tanramluk (b. 1979) is an Assistant Professor at the Institute of Molecular Biosciences, Mahidol University, and the Integrative Computational BioScience (ICBS) Center, where she leads groundbreaking research in machine learning, structural bioinformatics, and molecular design. She received a Ph.D. (Biochemistry) from the University of Cambridge. She is the lead developer of various AI-powered drug design platforms, e.g., MANORAA.org and Ligand.Cafe and MproCovid.com. Her contributions have earned her numerous recognitions, e.g., the Science and Sustainability Award from the British Council and the Top 100 in Chemistry from Nature Portfolio.

AI in Drug Discovery Research (S5-I-005)

Identification of USP2 dynamic pocket as a novel anticancer target

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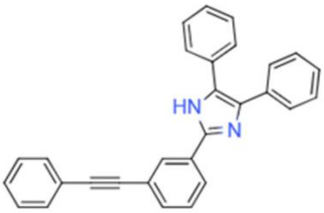
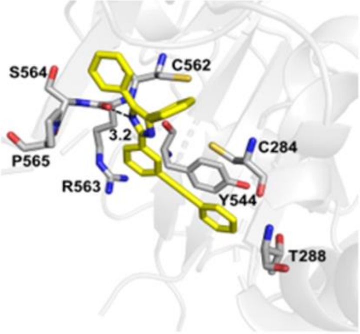
The natural product gambogic acid (GA) inhibits the deubiquitinating activity of ubiquitin-specific protease 2 (USP2) by forming a covalent bond with its Cys284 residue, leading to KRAS degradation and thereby suppressing the proliferation of multiple myeloma cells. In crystal structures, Cys284 is embedded within the protein's interior. Through molecular dynamics (umbrella sampling), we identified a conformational state where Cys284 becomes exposed, revealing a newly formed pocket. Virtual screening combined with activity assays targeting this pocket identified the non-covalent inhibitor ICU30, which significantly inhibits multiple myeloma cell growth. Our study demonstrates that the novel pocket in USP2 represents a promising therapeutic target. Inhibiting USP2 to induce KRAS degradation may offer a novel therapeutic strategy for cancers harboring KRAS mutations.

Keywords: USP2; gambogic acid; molecular dynamics; dynamic pocket; drug design



ICU30



Dr. Zhijian Xu (b. 1985) earned his Ph.D. from Shanghai Institute of Materia Medica, Chinese Academy of Sciences (SIMM) in 2012 and is currently a full professor at the SIMM. Specializing in molecular simulation and drug design, he develops innovative computational methods and applies them to drug discovery. With over 150 publications, including 4 papers cited >200 times, he has filed 50+ patents and holds 6 software copyrights.

AI in Drug Discovery Research (S5-I-008)

Cheminformatics-guided optimization of the antimalarial activity and physicochemical properties of 2,4-diaminopyrimidines

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Plasmodium falciparum (Pf) is the most common and most deadly cause of malaria in humans. Due to the development of drug resistant, newer drugs, or drugs acting at new targets. Here, we report the preparation of forty-eight new 2,4-diaminopyrimidine derivatives that have been designed to target Pf protein kinome. Cheminformatics and bioinformatics methods have been extensively used to guide the development of these new molecules in the form of bioinformatics to determine the most probable Pf kinases, molecular docking to PDB and homology molecules of the most probable targets and guide structure modification and QSAR/informatics to uncover the key molecular descriptors to enhance antimalarial activity, mammalian cytotoxicity and solubility.

All compounds were assessed in chloroquine-resistant Pf3D7 strain and mammalian cytotoxicity in HepG2 cell lines. Phosphate buffer solubility, MDCK permeability, and metabolic clearance in human and rat microsomes were also assessed. Compounds **68** and **69** showed good Pf IC_{50}s of 0.05 and 0.06 µM, respectively and good selectivity over the mammalian cell line with SI >100 fold. The compounds also demonstrated good aqueous solubilities of 989.7 and 1573 µg/mL, respectively and moderate clearance (~3 mL/min/g) and permeability (>60 nm/s).

Keywords: *Plasmodium falciparum*; cheminformatics; 2,4-diaminopyrimidines; Pf3D7 strain; MDCK permeability

Paul Gleeson was born in the Republic of Ireland in 1978. He obtained his M.Chem. and PhD degrees in 2000 and 2003, respectively, from, the University of Manchester, United Kingdom. He currently works as lecturer at King Mongkut's Institute of Technology Ladkrabang. His research interests lie in the field medicinal chemistry, spanning synthetic organic chemistry, physico-chemical property determination and computational modelling of drugs and their targets.

AI in Drug Discovery Research (S5-I-014)

Antimalarial activity prediction of enantiomeric cycloguanil analogues using extremely randomized trees and particle swarm optimized-support vector regression intelligent approaches

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A series of antimalarial drug analogues, 1-(4-chlorophenyl)-6,6-dimethyl-1,3,5-triazine-2,4-diamine (CYC), have shown effective inhibition of *Plasmodium falciparum* dihydrofolate reductase (*Pf*DHFR). These analogues possess an asymmetric carbon atom, offering two enantiomers, (*R*) and (*S*), which are mirror images and differ in their biological activities. The stereochemistry of these compounds has not been well-explored, though understanding the enantiomeric effects is crucial for assessing clinical safety and effectiveness. This study investigates the stereoselectivity of *Pf*DHFR towards the (*R*) and (*S*) enantiomers of CYC analogues through molecular docking and quantitative structure-activity relationship (QSAR) analysis. The 3D structures of 50 CYC analogues, in both enantiomeric forms, were optimized using density functional theory (M062X/6-31G(d,p)), and molecular descriptors were calculated using the Molecular Operating Environment (MOE) program. Docking studies revealed *Pf*DHFR's enantioselectivity: CYC analogues with alkyl chain substituents favored the (*R*) enantiomer, while those with phenol chain substituents preferred the (*S*) enantiomer. The QSAR model, developed using extremely randomized trees and particle swarm optimization-support vector regression (PSO-SVR), demonstrated strong predictive capability (R^2 = 0.94, Q2 = 0.77, R^2_test = 0.88). This study provides valuable insights into designing chiral antimalarial inhibitors, emphasizing the importance of enantiopure drugs to minimize side effects.

Keywords: antimalarial inhibitors; molecular docking; particle swarm optimization; protein-ligand interaction; support vector regression

Dr. Luckhana Lawtrakul completed her doctorate (Dr.rer.nat.) in Theoretical Biochemistry at the University of Vienna. She is currently an Associate Professor in the School of Bio-Chemical Engineering and Technology at Sirindhorn International Institute of Technology (SIIT), Thammasat University. Her research focuses on computer-aided molecular modeling and molecular design, structure-activity relationships, conformational analysis, molecular dynamics simulations, quantitative structure-activity relationships (QSAR), and host-guest chemistry of cyclodextrins.

AI in Drug Discovery Research (S5-I-021)

Drug discovery and hit to lead optimization of potent inhibitors as antituberculosis agents

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Tuberculosis (TB) caused by Mycobacterium tuberculosis continues to be a major cause of mortality and has become a current public health problem. With the continuously increasing epidemic of drug-resistant tuberculosis by the emergence of multidrug resistant tuberculosis, widespread extensive drug-resistance TB, there is an urgent need to develop novel therapeutics to treat TB. We have focused on *In silico* drug discovery platform including structure-based drug design and virtual screening, de novo design, Cheminformatics and database of Natural Products, protein-ligand interaction simulations, Molecular Dynamics simulations, drug-likeness analysis and ADME/T prediction to identify potentially inhibiting compounds targeting TB. A variety of compound libraries, ranging from natural product libraries up to commercially available libraries were virtually screened. Biochemical and molecular biological data of the target proteins in complex with their ligands are essential parts of our research. The X-ray crystal structures of lead compounds complexed with the enzyme targets have been carried out to understand the binding mode and crucial interactions of lead compounds for binding in the enzyme target. Compounds identified highly potent inhibitors have been used as the potential templates for rational design of a new series followed by chemical synthesis and biological assay, to optimize the lead compounds. The active compounds discovered from our works would be promising candidate molecules for further development as novel antituberculosis agents.

Keywords: tuberculosis (TB); drug-resistant TB; *in silico* drug discovery; molecular dynamics simulations; natural products

Pornpan Pungpo received her Ph.D.in Chemistry from Kasetsart University, Thailand. She is an Associate Professor in Chemistry at the Department of Chemistry, Faculty of Science, Ubon Ratchathani University. Her research area encompasses an in silico drug discovery platform for the discovery of novel inhibitors for TB treatment, as well as experimental platforms that include the evaluation of biological activities of discovered compounds and structural modifications to identify potentially inhibiting compounds. She received several major awards, including the L'Oréal-UNESCO For Women in Science Award (2010) and the CRS Silver Medal Award (2024).

Branding value in health products

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Branding plays an important role in consumer products market, anyhow, in Health Products Market, there's still some room to improve. 3 parts that needed to be addressed as key players in Health Products Market are as followings; 1. An importance of Branding ; How the Branding helps our products sell & survive in the market 2. Branding Structure (Branding In Brief) ;

- a. Brand Component (Brand Combination) : what is the key component in Branding
- b. Relationship between Brand - Product - Consumer (Mapping with Buying Decision Funnel)
- c. Brand Archetypes (Brand Guideline)

3. Samples of Brand in Action (Cases & Examples)

In Summary, for Health Products Market still has an area to improve for Branding. Understanding Branding will help us as a player in this market can sell the products to the right targets with the right messages.

Keywords: brand; customer; marketing; health products market

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-I-007)

Nutraceutical market in practice in Vietnam presented

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Vietnam is rapidly emerging as one of Southeast Asia’s most promising markets for nutraceuticals, driven by rising income levels, increased health awareness, and a growing aging population. The sector has seen double-digit growth in recent years, supported by strong consumer demand for preventive healthcare and functional foods.

This presentation will offer practical insights into how the nutraceutical market operates in Vietnam, including:

- Consumer Behaviour Trends: What drives buying decisions — from traditional herbal preferences to modern wellness trends.
- Distribution Landscape: The role of pharmacies, e-commerce platforms, MLM models, and health clinics in reaching end users.
- Regulatory Framework: Key steps for product registration, importation, and labeling compliance under Vietnam’s Ministry of Health.
- Market Entry Challenges: Common barriers such as registration delays, competition from domestic brands, and trust-building with local consumers.
- Opportunities for Foreign Firms: Growing appetite for high-quality, science-backed products; joint venture models; and local partnerships for manufacturing or distribution.

GT Innovation brings real-world experience in guiding international companies to localize, comply, and thrive in Vietnam. This session will not only map the market but also present actionable strategies for entering and scaling in the Vietnamese nutraceutical space.

Keywords: Vietnamese nutraceutical; customer; health products market trend

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-I-008)

Functional nutraceutical for appetite stimulation and gut health in companion animals- MEWLICIOUS

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MEWLICIOUS – A Functional Nutraceutical for Appetite Stimulation and Gut Health in Companion Animals MEWLICIOUS is a nutraceutical dietary supplement developed through the integration of animal nutrition, feeding behavior science, and gastrointestinal biology. It aims to address the issue of chronic inappetence, which is commonly observed in clinical practice particularly in 30–40% of senior cats and approximately 20–30% of dogs - often resulting from gut microbiota imbalance, stress, or poor sensory response to food aroma and texture. The product is delivered in a flexible 2-in-1 powdered format that can be transformed into a meal topper, creamy soup, or lickable treat, depending on each pet's behavioral preference. Its formulation includes a precise combination of functional bioactive ingredients designed to restore digestive balance, support immune function, and improve feeding experience.

● Synbiotics (CHITO-oligosaccharides, Lactobacillus acidophilus, Bacillus coagulans): This synergistic blend of prebiotics and probiotics modulates gut microbiota and strengthens mucosal immunity. CHITO-oligosaccharides (COS) are low molecular weight fibers known to promote beneficial lactic acid bacteria, improve villus structure, and modulate mucosal cytokines. *L.acidophilus* and *B. coagulans* contribute to barrier integrity and immune signaling, including increased IgA and IL-10 expression, while suppressing pathogens such as *E. coli*.

● Type II Marine Collagen: Derived from deep-sea fish, this bioavailable form ofcollagen promotes gut barrier repair, joint flexibility, and skin hydration. Its high glycine and hydroxyproline content supports collagen synthesis at the intestinal mucosa and articular cartilage, offering potential benefits for aging animals or those with gut inflammation and joint stiffness.

● Easily Digestible Fish-Based Protein and Egg-Derived Fats: These high-quality ingredients ensure superior palatability, digestibility, and nutrient uptake. Fish protein is rich in taurine and essential amino acids critical forfeline liver and heart function. Egg-derived fats provide phospholipids and omega-3 fatty acids (e.g., DHA), supporting cognitive health, skin and coat condition, and reducing intestinal inflammation. Developed under the principle of Holistic Nutritional Care, MEWLICIOUS does not only target physiological function but also addresses the behavioral and emotional aspects of feeding. By combining flavor science with targeted gut support, it represents a novel tool in preventive veterinary nutrition—suitable for use in clinical practice as well as in the premium companion animal food industry

Keywords: functional nutraceutical; appetite stimulation; gut health

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-I-009)

Microwave-assisted biosynthesis of quercetin-stabilized gold nanoparticles with enhanced antibacterial and catalytic properties

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In the past few years, substantial progress has been made in the field of microwave-assisted biosynthesis of gold nanoparticles (AuNPs) using quercetin (QT) as a natural reducing and stabilizing agent. This study explores the rapid and eco-friendly synthesis of AuNPs facilitated by microwave irradiation, offering a time-efficient alternative to conventional methods. The AuNPs were thoroughly characterized to confirm their morphology, size, crystalline structure, and surface plasmon resonance (SPR). The synthesized AuNPs were confirmed by visual color change from yellow to violet and characteristic SPR peak at 519 nm. Furthermore, XRD studies clearly confirmed the crystalline nature of the face-centered cubic structure of AuNPs. Moreover, TEM images reveal that the AuNPs were found to be more or less spherical and have a slightly variable morphology with an average diameter of 14 nm. The antibacterial properties of QT and AuNPs were evaluated against two different bacterial strains via *Staphylococcus aureus* and *Escherichia coli*, demonstrating significant activity, particularly due to the stabilizing effect of QT. Additionally, the catalytic efficiency of the AuNPs was evaluated by their ability to reduce 4-nitrophenol to 4-aminophenol, a model reaction for the catalytic activity. The results were promising, with the rate constant of QT-AuNPs determined to be 0.1016 s^{-1}. This work highlights the dual functionality of QT-mediated AuNPs in enhancing both antimicrobial and catalytic properties, contributing to their potential applications in the biomedical and environmental fields. This study highlights the dual role of QT-mediated AuNPs in enhancing antimicrobial and catalytic properties, paving the way for innovative applications in both the biomedical and environmental fields. The uniqueness lies in leveraging the natural properties of QT to simultaneously improve biological activity and catalytic efficiency, offering a sustainable and multifunctional QT-AuNP solution.

Keywords: quercetin-stabilized gold nanoparticles; antibacterial; catalytic properties

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-I-010)

Anthocyanin rich-berry extracts coated magnetic Fe_3O_4 bionanocomposites and their antibacterial activity

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The relentless evolution of antibiotic-resistant bacteria has made treating bacterial infections with conventional antibiotics increasingly difficult. Consequently, there is an urgent demand for innovative strategies that demonstrate exceptional antibacterial efficiency to effectively combat these resilient pathogens. This study aimed to investigate the efficiency of extraction of anthocyanins-coated iron oxide nanoparticles (Fe_3O_4 NPs) as an antibacterial agent against *Escherichia coli* and *Staphylococcus aureus*-902. The anthocyanins were extracted from three different berries: mulberry, blackberry, and blackcurrant. The Fe_3O_4NPs were synthesized using the co-precipitation method with $FeCl_2{\cdot}4H_2O$ and $FeCl_3{\cdot}6H_2O$ metal precursors. Furthermore, anthocyanins were coated onto the surface of Fe_3O_4 through a simple sonication process, followed by the freeze-drying, resulting in Fe_3O_4/bionano-composites (BNC). The mulberry, blackberry, and black currant-derived anthocyanins coated Fe_3O_4 were labelled as Fe_3O_4/MB, Fe_3O_4/BB, and Fe_3O_4/BC, respectively. The resulting Fe_3O_4/BNCs were analyzed using various spectroscopy and microscopic techniques. The XRD results showed that the Fe_3O_4/BNC formed a face-centred cubic structure, with particle size determined debye-Scherrer's equation, and the obtained particle size was 15–18 nm. Finally, the obtained Fe_3O_4/BNC was used as an antibacterial agent against *Escherichia coli* and *Staphylococcus aureus*-902. The Fe_3O_4/BNC exhibited strong antibacterial activity against bacterial species. Thus, this study offers a competitive approach to create recyclable antibacterial materials with specific antibacterial therapeutic properties.

Keywords: Fe_3O_4; anthocyains-rich; berry extracts; bio-nanocomposites; antibacterial activity; surface coating

Green synthesis of silver and gold nanoparticles using *Oroxylum indicum* plant extract for catalytic and antimicrobial activity

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This study highlights an eco-friendly microwave-assisted synthesis of colloidal silver (Ag°) and gold (Au°) nanoparticles, prepared using plant extract of *Oroxylum indicum* (Oi). Flavonoids present in the plant extracts act as stabilizing and reducing agents for synthesis of silver (Oi-AgNPs) and gold nanoparticles (Oi-AuNPs). The presence of flavonoids in plant extracts of Oi was confirmed by NMR and mass spectroscopy. The synthesized nanoparticles were analyzed by different characterization techniques. Surface plasmon (SPR) peaks appear at 403 nm (AgNPs) and 546 nm (AuNPs) in the UV-spectrum, revealing the formation of Oi-Ag and Oi-AuNPs. The size of the particles, as indicated by HRTEM analysis, was found to be 15 nm ± 3 nm (AgNPs) and 5.25 nm ± 1.00 nm (AuNPs). The resulting Oi-Ag and Oi-AuNPs exhibit face-centered cubic structures (FCC). Using Debye-Scherrer's equation, the average particles were 21 nm and 8 nm in diameter, respectively. The synthesized Oi-Ag and Oi-AuNPs are found to be extremely toxic against *Staphylococcus aureus* (*S. aureus*) and Escherichia coli (*E. coli*) bacteria. Furthermore, the catalytic efficiency of the prepared Oi-Ag and Oi-AuNPs were studied by the reduction of 4-nitrophenol. The obtained k_{obs} values were 0.12 s^{-1} for AgNPs and 0.22 s^{-1} for AuNPs, and these results reveal that the AuNPs are 2-fold more active than AgNPs. The obtained results illustrate that the prepared microwave-assisted green syn thesis of Ag and AuNPs is non-toxic and can be utilized for dual applications, including the reduction of 4-NP and serving as an efficient antibacterial agent. The reaction kinetics and recycling efficiency of the catalysts for the reduction of 4-NP were also examined. In conclusion, the Ag and AuNPs synthesized using the microwave-assisted biosynthesis method exhibit promising potential as catalysts for hydrogenation reactions and highly effective antimicrobial agents.

Keywords: silver nanoparticles; gold nanoparticles; *Oroxylum indicum*; 4-nitrophenol; antibacterial

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-I-012)

Plant waste as a silver nano catalyst: Assessing their application in bioremediation

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The release of organic dyes from food, textiles, plastic, leather, and printing industries into the environment is a rising issue which is impacting water quality, harming aquatic life, and potentially posing health risks to humans. Azo dyes contain one or more azo bonds providing them with high stability and potent colouring ability. Azo bonds are chemically and photolitically stabilized xenobiotics. Hence, they can withstand natural degradation. The unorganized degradation of azo bonds produces toxic aromatic amines causing induced health hazards to humans and harm to aqua systems. Moreover, para-nitrophenol (PNP) is another organic compound industrially used for various purposes including pharmaceuticals, insecticides, and explosives. The high stability and solubility of these compounds provide them with resistance to natural oxidation. Numerous efforts such as microbial treatment, chemical oxidation, precipitation, and adsorption, including catalyzed degradation have been employed to remove azo dyes and PNP from wastewater. These traditional degradation methods are time and cost-consuming. This triggered the researchers to study a novel and effective degradation methodology. As a result, photocatalysis was regarded as a favourable process for degradation of azo dyes. In 1978, it was discovered that silver nanoparticles (AgNPs) have excellent photoresponsivity and are efficient photocatalysts. Nanotechnology, which involves the use of nanomaterials for the benefit of humans, has become extremely advanced over the past decades and is now employed in several industries such as pharmaceuticals, cosmetics, textiles, food, and agriculture. This study focuses on synthesis of AgNPs using waste products of plant varieties and assessing the bioremediation potential. The finding showed that the synthesised AgNPs completely degraded azo dyes by breaking the -N=N- into amines without producing toxic or secondary components. Additionally, the complete catalytic degradation of p-nitrophenol into p-aminophenol is evident. This study thereby concludes that the synthesized AgNPs can be utilized in bioremediation of environmental pollutants, through a cost-effective, and environmental-friendly alternative.

Keywords: bioremediation; silver nanoparticle; catalysis, photocatalysis; azo-dye, para-nitrophenol

Magnetic duckweed-derived adsorbent for efficient methylene blue removal: A green and cost-effective approach

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This study investigates the synthesis and characterization of a magnetic duckweed (MDW)-derived adsorbent using a green reducing agent, ascorbic acid (AA) as a reducing agent for the efficient removal of methylene blue (MB) from aqueous solutions. This novel MDW was synthesized via a simple co-precipitation method, incorporating magnetite nanoparticles (NPs) of Fe_3O_4 onto the DW matrix. The MDW achieved a maximum MB adsorption capacity of 78.59 mg/g. The optimal adsorption conditions were determined as follows: pH 10, initial MB concentration of 50 mg/L, contact time of 60 min, and an adsorbent dosage of 10 mg, achieving a maximum removal efficiency of 85.27%. The adsorption process followed pseudo-second-order (PSO) kinetics, indicating chemisorption as the rate-controlling step. Isotherm studies revealed that MB adsorption was best described by the Temkin model, suggesting a heterogeneous adsorption surface with multi-layer interactions. Thermodynamic analysis confirmed an exothermic and spontaneous process, with negative Gibbs free energy ($\Delta G°$) values, indicating favorable adsorption at lower temperatures driven by electrostatic interactions, π–π interactions, and hydrogen bonding. Cost analysis revealed a synthesis cost of approximately RM 29.51/kg using abundant and eco-friendly raw materials and method. Optimization studies demonstrated that adsorption efficiency was significantly influenced by adsorbent dosage, initial dye concentration, and pH, with the highest removal efficiency observed under alkaline conditions. Regeneration experiments confirmed the material's reusability, retaining over 69% removal efficiency after five cycles. These results highlight MDW as a sustainable, low-cost, and efficient adsorbent for dye-contaminated wastewater treatment, offering a promising solution to environmental pollution challenges.

Keywords: duckweed; magnetite, adsorbent; methylene blue; adsorption kinetics

Vin Lim Teik Zheng received his B.Sc (Hons) Chemistry (UPM), M.Sc in Analytical Chemistry (UPM), Ph.D in Material Chemistry (Kyutech). At present, he is a senior lecturer at Universiti Putra Malaysia Bintulu Campus. His research focuses on adsorption and photocatalytic remediation of noxious pollutants using graphene based materials. Green synthesis of nanomaterials for wastewater treatment.

Green Chemistry; Paving the Way to a Sustainable Future (S8-I-012)

Next-gen molecular design: Integrating quantum computing, AI, computer-aided molecular design (CAMD) and blockchain for a sustainable future in healthcare, energy, and the environment

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The convergence of quantum computing, artificial intelligence (AI), computer-aided molecular design (CAMD), and blockchain technologies is redefining the future of molecular innovation across healthcare, energy, and environmental sustainability. This talk highlights how emerging digital tools are redefining the molecular innovation pipeline from early-stage design to real-world application by integrating quantum-enhanced algorithms, deep learning models, and physics-informed simulations. In healthcare, the integration of quantum-enhanced simulations with AI-driven prediction models is enabling the rapid identification and optimization of drug candidates tailored to individual patient profiles. Blockchain ensures the secure handling of sensitive biomedical data, supporting trusted collaboration and regulatory compliance in precision medicine. In energy and materials science, quantum-AI systems guide the design of novel catalysts, batteries, and functional materials with minimal environmental footprint while blockchain networks facilitate provenance tracking and decentralized verification of research data and supply chains. Environmental applications are further strengthened through CAMD-led green chemistry initiatives, where blockchain supports the traceable life cycle of sustainable materials, contributing to circular economy models and carbon accountability. Together, these technologies offer a digital backbone for mol ecular systems engineering that is efficient, ethical, and scalable.This presentation emphasizes how the intersection of quantum intelligence, AI, and blockchain provides a robust, interdisciplinary foundation for accelerating scientific advancement while ensuring the ethical, secure, and equitable delivery of solutions that address global sustainability challenges.

Keywords: artificial Intelligence (AI); blockchain technology; molecular design; sustainability and green chemistry

Dr. Vannajan Sanghiran Lee received the 2023 UNESCO Woman of Influence in Science and Technology for her groundbreaking work in molecular modeling and quantum science. She leads the Centre of Excellence for Quantum Information Science and Technology (UMQIST) at Universiti Malaya. She plays a key role in shaping the future of quantum research and education in the region. Dr. Lee, a former DPST scholarship at Chiang Mai University, earned her Ph.D. from the University of Missouri–Kansas City in 2001. She continues to advance frontier science through her leadership in MolDesign and Qubios Sdn. Bhd.

Green Chemistry; Paving the Way to a Sustainable Future (S8-I-021)

Environmental benign materials through ligno-cellulose

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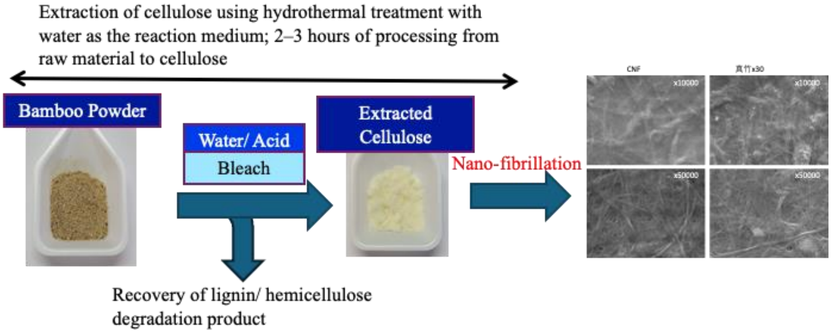
The growing demand for sustainable alternatives to petroleum-based plastics has underscored the importance of biomass-derived materials. Although bamboo, oil palm residues, and other agricultural wastes have high carbon fixation potential and are regionally abundant, they remain largely underutilized. Our research develops an environmentally responsible process that separates cellulose and lignin from diverse lignocellulosic feedstocks via one-step hydrothermal fractionation with dilute nitric acid (HNO_3). This solvent-free method enables high-yield cellulose extraction with enhanced crystallinity and simultaneously recovers hemicellulose and lignin derivatives. The extracted cellulose can be converted into value-added materials such as cellulose nanofibers (CNFs) through fibrillation or surface modification. While CNFs tend to aggregate in hydrophobic polymers, well-dispersed CNFs can act as strong reinforcing fillers comparable to glass or carbon fibers. These materials are promising for use in biodegradable packaging, composites, and flame-retardant systems. The process is adaptable to various biomass types, improving scalability and practical application. By leveraging this technology, we can design renewable-resource-based materials with biodegradability and recyclability in mind. This research contributes to sustainability by advancing biomass utilization, reducing fossil dependence, and enabling a circular, low-carbon material economy.

Keywords: hydrothermal reaction; biomass valorization; cellulose; lignin; sustainable materials



Dr. Yoshito Ando (published as Yoshito Andou), Ph.D. in Engineering, is an Associate Professor at Kyushu Institute of Technology and the Director of the Collaborative Research Centre for Green Materials on Environmental Technology. His research focuses on sustainable materials, especially the extraction and functionalization of cellulose and lignin from unused lignocellulosic biomass such as bamboo.

Green Chemistry; Paving the Way to a Sustainable Future (S8-I-022)

Sustainable esterification technique for bio-based cellulose esters production

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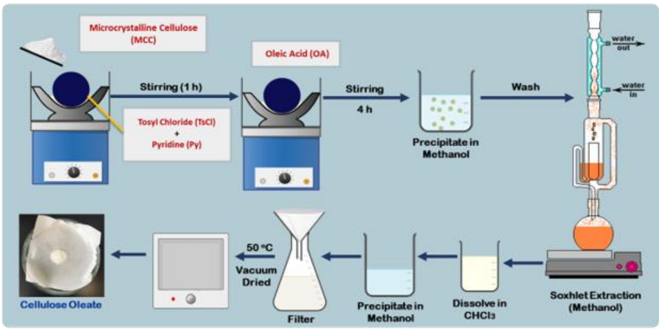
Cellulose, the most abundant natural polymer, holds significant potential as a sustainable alternative to petroleum-based polymers. Due to its rich abundance of hydroxyl groups, it offers a versatile platform for the development of novel materials. In this study, esterification method was explored to synthesize cellulose esters through both conventional chemical processes and a mechanochemical approach. The differences in reactivity and resulting properties of the modified celluloses were systematically investigated. X-ray diffraction (XRD) analysis revealed that the mechanochemically synthesized cellulose esters exhibited a semi-crystalline structure, whereas those produced via chemical esterification were predominantly amorphous. Additionally, the modification introduced thermoplastic characteristics to the cellulose. Among the samples, cellulose oleate prepared by chemical esterification (C_CO) achieved the highest degree of substitution (DS) at 2.67. Interestingly, cellulose esters with a lower DS demonstrated superior tensile strength. Overall, this eco-friendly esterification strategy offers a promising alternative to traditional methods by reducing solvent use and enhancing environmental sustainability.

Keywords: cellulose modification; cellulose plastic; mechanochemical esterification; sustainable; cellulose esters



Jacqueline Lease is an Assistant Professor at the Advanced Research Headquarters, Research Center for Focal Project, Collaborative Research Center for Green Materials on Environmental Technology, Kyushu Institute of Technology, Japan. She received her Master's degree in Engineering from Kyushu Institute of Technology. Currently, her research focuses on the modification of cellulose and the development of cellulose derivatives. Her broader research interests include green chemistry, materials engineering, and polymer chemistry, with a particular emphasis on environmentally sustainable materials and technologies.

Green Chemistry; Paving the Way to a Sustainable Future (S8-I-023)

Recent advances in the catalytic conversion of bioethanol to green chemicals over heterogeneous catalysts

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Bioethanol is a renewable feedstock derived from the fermentation of biomass such as molasse, casava, corn, etc. At present, the major use of ethanol is an additive in gasoline to produce gasohol. To reduce the greenhouse gas, the usage of electric vehicles (EV) will remarkably increase resulting in less usage of oil-based vehicles. Therefore, in the near future, the ethanol consumption will also dramatically decrease. It is crucial to find the strategy to utilize ethanol efficiently. The thermochemical conversion of ethanol to other chemicals is an alternative solution. It has been the focus of our research group for a decade. Ethylene and diethyl ether can be obtained via catalytic dehydration of ethanol using solid acid catalysts, such as alumina, beta-zeolite, and WO_3-supported catalysts. The dehydrogenation of ethanol can produce acetaldehyde and hydrogen using activated carbons and Cu-based supported catalysts. Esterification of ethanol and suitable carboxylic acids can produce esters such as ethyl propanoate and ethyl lactate, which can be used as green solvent. The development of biomass-derived solid acid catalysts for esterification of ethanol is also investigated.

Keywords: bioethanol; solid catalyst; dehydration; dehydrogenation; esterification

Bunjerd Jongsomjit received his Ph.D. (Chemical Engineering) from the University of Pittsburgh, USA. He is presently a professor in the Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University. His research focuses on heterogeneous catalysis involving catalytic ethanol conversion and olefin polymerization catalysts. He received the Catalysis Development Excellence Award (The Asian-Pacific Association of Catalysis Societies, APCAT-9) in 2023.

Ryoji Noyori ACES Awards Symposium (S9-I-001)

Synthesis with boron at the helm

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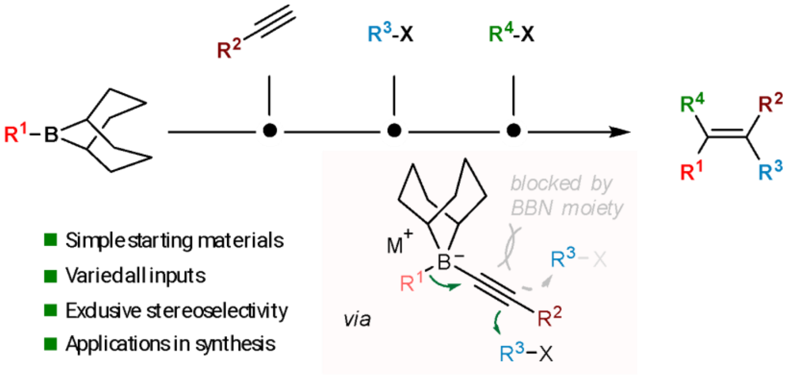
Cross coupling, particularly Suzuki cross coupling, is one of the most important reactions in medicinal chemistry. Most couplings involve sp2-sp2 bond formation but this invariably leads to flat molecules. With increasing interest in accessing three dimensional space (escape from flatland), there is increasing interest in broadening this coupling reaction to include sp2-sp3 and even sp3-sp3 coupling. In this lecture I will show how new variations of the Zweifel olefination reaction enable sp2-sp3 couplings (alkenes with alkyl boronic esters) and an extension of this reaction which enable aromatics to be coupled with hindered secondary and even tertiary boronic esters. I will also discuss how this chemistry can be applied to the stereocontrolled synthesis of tetrasubstituted alkenes and how we can even extend this work to stereocontrolled sp3-sp3 couplings, where stereochemistry can essentially be dialled in.

Keywords: Boron; asymmetric synthesis; natural products



Varinder K. Aggarwal studied chemistry at Cambridge University and received his Ph.D. in 1986 under the guidance of Dr. Stuart Warren. After postdoctoral studies (1986-1988) under Prof. Gilbert Stork, Columbia University, he returned to the UK as a Lecturer at Bath University. In 1991 he moved to Sheffield University, where he was promoted to Professor in 1997. In 2000 he moved to Bristol University where he holds the Chair in Synthetic Chemistry. He has received numerous awards including RSC Perkin Award 2013; RS Davy Medal 2019, and he was elected Fellow of the Royal Society in 2012.

Ryoji Noyori ACES Awards Symposium (S9-I-002)

Developing new synthetic methodologies of dearomatization reactions

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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: aromatic compounds; asymmetric catalysis; dearomatization; homogenous catalysis; synthetic reaction

Shu-Li You was born in Henan, China (1975), and received his BSc in chemistry from Nankai Univ. (1996). He obtained his PhD from SIOC in 2001 under the supervision of Prof. Lixin Dai before carrying out postdoctoral studies with Prof. Jeffery Kelly at The Scripps Research Institute. From 2004, he worked at the Genomics Institute of the Novartis Research Foundation as a PI before returning to SIOC as a Professor in 2006. His research interests mainly focus on asymmetric C-H functionalization and catalytic asymmetric dearomatization reactions. He is the recipient of RSC Merck Award (2015) and Yoshida Prize (2024). Prof. You has been an Associate Editor for JACS since 2021.

Ryoji Noyori ACES Awards Symposium (S9-I-003)

Transition metal enolate chemistry: Past, present, and future

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We have been working on chiral late transition metal enolate chemistry for many years. We discovered that chiral palladium enolates act as mild nucleophiles and developed Pd-catalyzed enantioselective reactions between various carbonyl compounds and electrophiles. [e.g. *J. Am. Chem. Soc.*, **1998**, *120*, 2474; **1999**, *121*, 5450; **2002**, *124*, 11240; **2002**, *124*, 14530; **2005**, *127*, 10164; **2006**, *128*, 14010]. The origin of the excellent enantioselectivity can be simply explained by the steric repulsion between the stable square planar Pd(II)-bisphosphine enolate complex and the electrophile. [*Tetrahedron* **2015**, *71*, 6594 and references cited therein] Recently, we have focused on the asymmetric reactions mediated by Ni(II) enolate complexes. We have developed highly enantio- and diastereo-selective reactions of α-ketoesters catalyzed by a Ni(II)-diamine complex. [e.g. *J. Am. Chem. Soc.* **2010**, *132*, 4036; *Nature Comm.* **2017**, 8, 14875; *J. Am. Chem. Soc.* **2017**, *139*, 8661; *J. Am. Chem. Soc.* **2021**, *143*, 9094] A mechanistic study revealed the dynamic features of the Ni complex and completely different principle of the asymmetric induction. We have recently also become interested in the reactions of α-carbonyl radicals. [*ACS Cat.* **2020**, *10*, 12770; *Angew. Chem. Int. Ed.* **2024**, *63*, e202405876). In addition to these catalytic reactions, the late transition metal enolate chemistry could contribute to chemical biology. I would also like to present the preliminary results of these new area of research. [*Chem. Sci.* **2023**, *14*, 8249]

Keywords: late transition metal enolate; asymmetric reaction; palladium; nickel

Born in 1959 and graduated from Chiba University (B. 1981, M. 1983, PhD 1989). Employments: Researcher, Sagami Chemical Research Center (SCRC, 1983-1986), Research Associate, Hokkaido University (1986-1990), Postdoctoral fellow, Harvard University (1990-1992), Assistant Professor, University of Tokyo (1992-1995), Group Leader, SCRC (1996-1999), Associate Professor, University of Tokyo (1999-2000), Professor, Tohoku University (2000-2006), Chief Scientist/Group Director, RIKEN (2006-), Director, RIKEN Center for Sustainable Resource Science (2025-). Representative Awards: The Chemical Society of Japan Award for Creative Work, Synthetic Organic Chemistry Award, Japan, Arthur C. Cope Scholar Award, The Pharmaceutical Society of Japan Award, Medal of Honor with Purple Ribbon.

Ryoji Noyori ACES Awards Symposium (S9-I-004)

Spin states matter - fundamentals, applications and translation to drug discovery

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University of Bayreuth, Organic Chemistry II, Universitätsstr. 30, 95447 Bayreuth, Germany
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Carbenes and nitrenes are versatile reactive intermediates that find widespread application in organic synthesis. Their high reactivity, however, often necessitates the use of metal complexes for stabilization of such species. [*Chem. Rev.* **2015**, *115*, 9981; *Chem. Commun.* **2022**, *58*, 2788]

Herein, we describe our recent approaches towards photochemical and photocatalytic carbene and nitrene transfer reactions. Strategies in accessing either singlet or triplet carbenes will be discussed and their applications in synthesis methodology will be presented. [*Angew. Chem. Int. Ed.* **2021**, *60*, 13271–13279; *Angew. Chem. Int. Ed.* **2022**, *61*, e202111892]

We commence with a discussion of nitrene intermediates and how these can be accessed under visible light irradiation without the need of conventional metal catalysts. We describe strategies, how the access of nitrene intermediates can be manipulated by single electron transfer reactions or direct photoexcitation. [*Nature Commun.* **2022**, *13*, 86] We conclude with a discussion of a collaborative approach towards drug discovery, where fundamental discoveries can be translated into new drugs and medicines. [*Science*, **2024**, *383*, 498–503]

Keywords: photochemistry; photocatalysis; carbenes; nitrenes; cycloaddition

Rene M. Koenigs studied chemistry at Goethe University, Frankfurt/M. (Germany) and performed his PhD under the supervision of Magnus Rueping. Following a postdoctoral stay at the pharmaceutical company Grunenthal, he started his independent career as assistant professor at RWTH Aachen University in 2015 and got promoted to Full Professor in 2022. Since April 2025, he holds a Chair Professor position at University of Bayreuth. His main research areas focus on carbene and nitrene chemistry and their application to organic synthesis methodology and drug discovery.

Ryoji Noyori ACES Awards Symposium (S9-I-005)

Stereodivergence in catalytic asymmetric conjugate additions

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Catalytic asymmetric conjugate additions of carbon nucleophiles have become a powerful method for constructing multi-stereogenic molecules with precise stereochemical control. Our group focuses on developing strategies to selectively access diverse diastereomeric conjugate-addition products through carbon–carbon bond formation. Key approaches for controlling the stereochemical outcomes of these reactions include altering alkene geometry, synergistic catalysis, and isomerization of conjugate adducts. These methods enable the efficient generation of various 1,5-functionalized compounds, which serve as versatile building blocks for synthesizing complex chiral molecules. Specifically, we have developed stereodivergent strategies to direct the formation of two or three contiguous stereocenters, some involving a phosphorus-based stereogenic center, in acyclic systems. In this presentation, I will discuss our recent advancements in these areas.

Keywords: stereodivergence; asymmetric catalysis; P-stereogenic center; multiple stereocenters; conjugate addition

Sarah was born in 1986. She received her BS from KAIST (2009) and Ph.D. from MIT (2014), followed by an NIH Postdoctoral Fellowship at UC Berkeley (2015-2017). She served as assistant/associate professor at Yonsei University (2018.03-2025.02) and is now associate professor at KAIST (2025.03~present). She has received several fellowships and awards, including the KCS-Wiley Young Chemist Award and Young Organic Chemist Award (2023). She also serves on the Early Career Advisory Board of the journals such as Asian Journal of Organic Chemistry, Science of Synthesis, and Organic Chemistry Frontiers.

Ryoji Noyori ACES Awards Symposium (S9-I-006)

Multifunctional chemical biology tools: Advances in synthetic strategies for small molecules and bioconjugates

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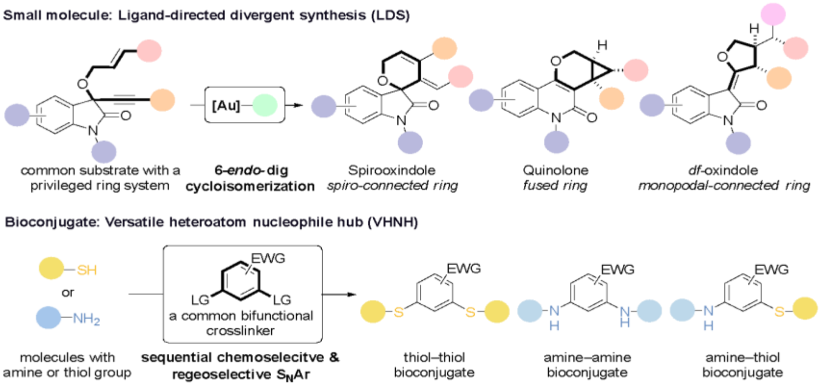
The advancement of chemical biology is driven by the development of efficient synthetic strategies and functional molecular tools. Our group focuses on the design of chemical biology platforms that address diverse molecular synthetic challenges through streamlined yet highly effective chemical approaches. Two multifunctional chemical biology tools will be presented. The first is a ligand-directed divergent synthesis (LDS) strategy, which enables the generation of structurally diverse small-molecules via a single catalytic transformation modulated by ligand variation. Based on this approach, three structurally distinct scaffolds—spirooxindole, quinolone, and *df*-oxindole—were synthesized from a common oxindole-derived 1,6-enyne substrate. The second tool is a versatile heteroatom nucleophile hub (VHNH), constructed from a common electron-deficient arene scaffold that functions as a bifunctional crosslinker. Through sequential chemo- and regioselective nucleophilic aromatic substitution (S_NAr) reactions, this platform enables the modular construction of thiol–thiol, amine–amine, and thiol–amine bioconjugates. Collectively, these synthetic methodologies offer general and modular platforms for the development of broadly applicable tools in chemical biology.

Keywords: divergent library synthesis; bioconjugation; chemical protein modification



Yen-Chun Lee (b. 1986)
2018 Ph.D. Dept. of Chemical Biology, Max Planck Institute (MPI) Dortmund, DE.
2018-2021 DFG research fellow, Dept. of Chemistry, Massachusetts Institute of Technology (MIT), USA.
2021-current Assistant Professor Dept. of Chemistry, National Cheng Kung University (NCKU), TW (2021-present).
Area of research: chemical biology, organic chemistry, peptide chemistry.

Ryoji Noyori ACES Awards Symposium (S9-I-007)

Exo-selective intramolecular (4+3) cycloadditions of epoxy enolsilanes

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Pauline Chiu[1,2,3,*]
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[3]*Laboratory for Synthetic Chemistry and Chemical Biology Limited, Hong Kong Science Park, Hong Kong, P. R. China*
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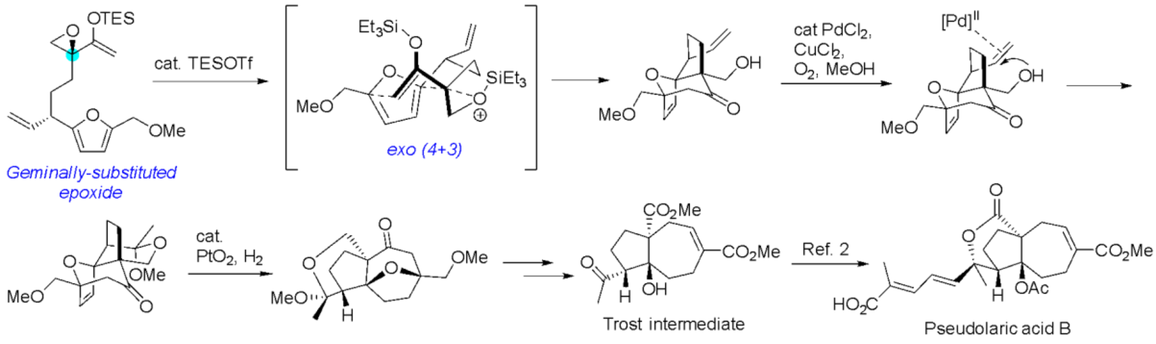
The intramolecular (4+3) cycloaddition of a new class of epoxy enolsilane substrates, whose epoxides are geminally-substituted on the tether to the furan, generate *trans*-fused perhydroazulene frameworks. [*ChemrXiv,* doi:10.26434/chemrxiv-2025-d0vx2] The reaction is highly diastereoselective in the exo-mode, as opposed to cycloadditions of previous vicinally-substituted substrate types.

Using this intramolecular cycloaddition as the key reaction, a key intermediate in Trost's synthesis of pseudolaric acid B was accomplished, [*J. Am. Chem. Soc.* **2007**, *129*, 14556] representing the shortest asymmetric synthesis of this anti-tumor natural product to date.

Keywords: cycloaddition; perhydroazulenes; pseudolaric acid; natural product



Pauline Chiu (b. 1964) received her PhD in 1993 from the University of Toronto with Mark Lautens. After postdoctoral studies (1994–1995) with Samuel J. Danishefsky at Columbia University, she joined the University of Hong Kong and became Full Professor in the Department of Chemistry in 2011. Her research is in the development of synthetic methodology and their applications to the synthesis of natural products. She has served as Associate Editor of Organic Letters (2018–2024) and is a Board member of Organic Syntheses (2021–). She is also currently the Associate Vice-President of Teaching and Learning at the University of Hong Kong.

Young Career Development under FACS-ACS Collaboration (SA-I-002)

Horizon Europe strategic plan 2025–2027: Unlocking opportunities for collaboration in research funding

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This session provides an in-depth overview of the Horizon Europe Strategic Plan for 2025–2027, highlighting its objectives and strategic priorities, along with opportunities for research engagement within this extensive funding framework. As part of the EURAXESS initiative, EURAXESS ASEAN plays a vital role in connecting researchers and institutions across ASEAN and Europe, promoting Horizon Europe—EU's flagship research and innovation program with over €95 billion in funding. In 2024, ASEAN participation saw notable growth, with signed grants increasing from 87 to 115 and total participants rising from 106 to 134 since 2021. Horizon Europe has significantly contributed to advancing scientific knowledge and addressing global challenges such as climate change, biodiversity loss, and digital transformation. Amid escalating geopolitical tensions and global crises, the program's strategic importance is heightened, emphasizing the EU's commitment to green and digital missions. The plan aligns with the European Green Deal's objectives and the urgent need for scientific innovation to confront climate and societal challenges, especially considering Europe's status as the fastest-warming continent. Participants will gain insight into the specific opportunities within Pillar I—focusing on excellent science—and Pillar II—addressing global challenges and boosting European industry competitiveness. This session aims to empower researchers and institutions to actively engage with Horizon Europe's strategic agenda, fostering enhanced collaboration, innovation, and societal progress across the ASEAN-EU research community.

Keywords: Horizon Europe; MSCA; ERC; Pillar II; ASEAN-EU research cooperation

KRMH Tatas Brotosudarmo, Ph.D. (born 1981) is a biochemistry at Petra Christian University, Indonesia, specializing in food chemistry and analysis. He holds a Ph.D. from the University of Glasgow and a master's from Ludwig-Maximilian University, Munich. As EURAXESS Worldwide Representative for ASEAN, he promotes EU-ASEAN research collaborations, focusing on Horizon Europe and researcher mobility. Recognized with awards including the Georg Foster Fellowship from the Alexander von Humboldt Foundation (2019) and the Toray Science & Technology Award (2017), he has led initiatives to strengthen international research networks and innovation in Southeast Asia.

Young Career Development under FACS-ACS Collaboration (SA-I-003)

Cross-cultural perspectives on becoming an outstanding scientist

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In today's interconnected world, being an outstanding scientist is about more than mastering technical skills. It's also about understanding people, navigating different cultures, collaborating across disciplines, and growing together through shared experiences. This session invites you to explore what it truly means to be a scientist through the lens of diverse cultural values, educational journeys, and personal stories. We'll look at how our backgrounds shape the way we think, solve problems, and communicate and how these differences can strengthen scientific discovery. We'll also spotlight the efforts of student-led groups like the ACS Malaysia Chapter, which plays a vital role in supporting young scientists. From outreach and mentorship to leadership training and international connections, these initiatives help students not just build careers, but grow into thoughtful, globally minded changemakers. By sharing real stories and reflections, we hope to inspire a more inclusive, compassionate vision of scientific excellence—one that values who we are as much as what we know.

Keywords: cross-cultural collaboration; diversity in science; STEM education; student scientific leadership; ACS Malaysia chapter

Dr. Vannajan Sanghiran Lee received the 2023 UNESCO Woman of Influence in Science and Technology for her groundbreaking work in molecular modeling and quantum science. She leads the Centre of Excellence for Quantum Information Science and Technology (UMQIST) at Universiti Malaya. She plays a key role in shaping the future of quantum research and education in the region. Dr. Lee, a former DPST scholarship at Chiang Mai University, earned her Ph.D. from the University of Missouri–Kansas City in 2001. She continues to advance frontier science through her leadership in MolDesign and Qubios Sdn. Bhd.

Young Career Development under FACS-ACS Collaboration (SA-I-004)

Your career compass: Guidelines for success and pitfalls to avoid

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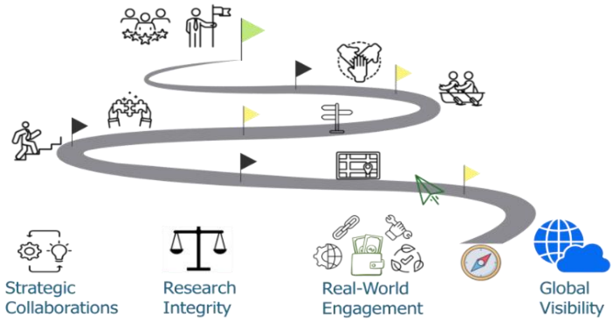
Navigating a successful career in science requires strategic thinking, meaningful collaborations, research integrity, and alignment with real-world needs. This presentation provides early-career chemists with essential guidelines to build impactful careers while avoiding common pitfalls. The talk explores four critical success pillars: strategic collaborations across disciplines, real-world engagement addressing market demands, research integrity as a career cornerstone, and adapting practices to meet societal challenges. Emphasis is placed on maintaining awareness of global demand and emerging trends while building visibility at national and international levels through conferences, professional societies, and collaborative networks. Drawing from successful career trajectories and common missteps, this presentation offers practical advice for young professionals. Attendees will learn to recognize collaboration opportunities, engage diverse audiences, uphold ethical standards, align work with global needs, and strategically build professional recognition. The talk will address the **ACS Thailand Chapter**'s practical roadmap tailored to help young researchers−whether in universities or research centers−navigate their unique environments and accelerate their development into impactful scientific leaders.

Keywords: Career development, Research integrity, Global collaboration, Professional visibility, ACS Thailand Chapter



Siwaporn Meejoo Smith (born 1976) is a Professor of Materials Technology at Mahidol University, Acting Deputy Director at the National Nanotechnology Center (Thailand), and Chair of ACS Thailand Chapter. She earned her Ph.D. in Chemistry from the University of Birmingham (UK.) She has been recognized with the 2015 L'Oréal Thailand For Women in Science Fellowship, highlighting her contribution to green technologies for the environment. Passionate about driving research into real-world applications, Siwaporn actively help researchers to translate their work into solutions with local and global impact.

TU-Frontier Lab-JEOL joint session Contaminants of Emerging Concern: PFAS & Microplastics (SB-I-003)

Ocean microplastic pollution, current status and future view from the Atlas of Ocean Microplastic (AOMI) database

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The standardization/harmonization of measurements of microplastic abundance should be prioritized to compare/synthesize the data obtained by different researchers worldwide. Thereby, the effort to standardize microplastic measurements/analyses has been continued since the mid 2010's; see Michida et al. (2019) and GESAMP (2019) for guidelines supported by research works such as an interlaboratory comparison exercise to compare the numbers of man-made microplastics (Isobe et al., 2019). In 2024, we opened a database of microplastic abundance in the upper oceans via the Internet. This on-going project sponsored by the Ministry of Environment, Japan, was launched last year to create the database (Atlas of Ocean MIcroplastics; AOMI means 'blue ocean' in Japanese; https://aomi.env.go.jp/), where abundance data of microplastics collected mostly by surface net sampling across the world's ocean to date were archived. More than 13,500 sampling data were currently processed to multilevel datasets in line with the data processing in Isobe et al. (2021, 1:16, Microplastics & Nanoplastics). Using the database, the abundance of microplastics in the current and future oceans predicted by numerical model approach will be introduced in the presentation.

Keywords: microplastics; AOMI; oceans

Atsuhiko Isobe is a professor at the Research Institute for Applied Mechanics at Kyushu University. After graduating Ehime University, He had worked at the National Fisheries University as a research associate, Kyushu University as an associate professor, and Center for Marine Environmental Studies, Ehime University as a professor. He was awarded the Environment Minister's prize in 2018, the Prime Minister's prize in 2019, and the Prize for Science and Technology from the Minister of Education, Culture, Sports, Science and Technology in 2020, Japan Oceanographic Society award in 2025, for his marine plastic pollution research.

TU-Frontier Lab-JEOL joint session Contaminants of Emerging Concern: PFAS & Microplastics (SB-I-004)

Advanced polymer analysis with GC-HRTOFMS and AI-based software solutions

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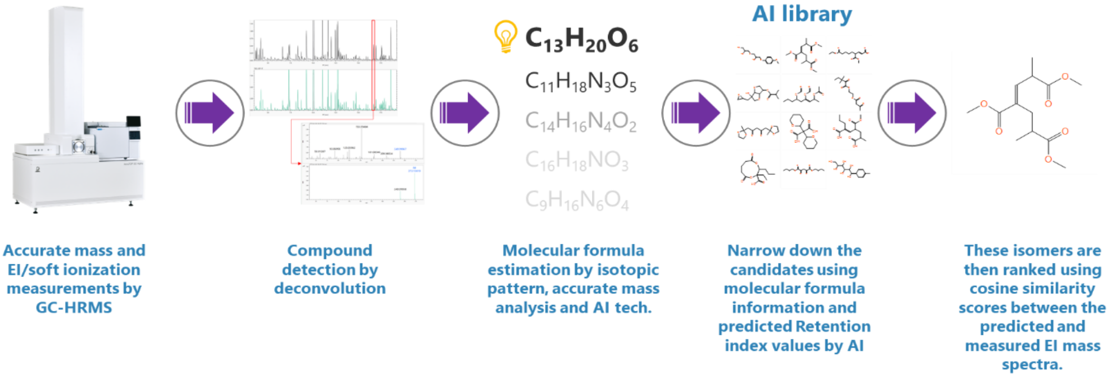
We have developed a machine learning model capable of predicting EI mass spectra from chemical structures. This prediction model was trained using the NIST23 mass spectral database. Using the trained model, we generated a predicted EI mass spectral database for over 100 million chemical compounds from PubChem, as well as over 100 million in silico compounds, including polymer pyrolyzates and trimethylsilyl (TMS) derivatives. We also developed a novel library search method to handle this vast database of approximately 200 million compounds with improved accuracy and efficiency. To enhance search efficiency, we first narrow down the candidate structures using the molecular formula of each discovered compound. Molecular formulae are best determined using both EI and soft ionization techniques, such as field ionization (FI), and the elemental compositions are calculated based on accurate mass measurements. This approach allows us to reduce the candidate pool from 200 million to a set of structural isomers. This newly developed structural analysis workflow, which leverages machine learning, is a powerful tool for qualitative GC-MS analysis, particularly in non-targeted screening applications.

Keywords: GC-MS; machine learning; EI mass spectral library; high mass resolution; soft ionization



Masaaki Ubukata received his Ph.D. in Engineering from Yokohama National University in 2008. He is currently the Manager of the Mass Spectrometry Application Group at JEOL, where he has worked for over 20 years as a specialist in mass spectrometry. Hehas published more than 20 papers related with mass spectrometry.

TU-Frontier Lab-JEOL joint session Contaminants of Emerging Concern: PFAS & Microplastics (SB-I-005)

Enhancing the analytical performance of microplastic in water sample

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Micro and nano plastics (MNPs) have been become a big global issue due to effect on human health. The waste plastic degraded to small size and distributed to ecosystem. The living things contain plastic inside. The analysis of MNPs in environmental samples are necessary. However, the detection limit has been still needed to overcome. The improvement of efficiency of MNPs analysis is a challenge. This research presents the application of adsorbent material especially mesoporous silica to increase the collecting of MNPs in water sample. In this study, MNPs are identified and quantified using pyrolysis gas chromatography-mass spectrometry (PY-GC/MS). Surface water (SW) sample at Thammasat University Pattaya center was pretreated by density separation using 1.8 g.cm^{-3} $ZnCl_2$ solution, followed by adsorption with SBA-15 and then vacuum filtration through 1.2 µm glass microfiber filters. The results revealed that the proposed method could detect MNPs in environmental water, among all plastic types, PVC, SBR, PC, PET, and N6 were the dominant polymer types from samples without and with adsorbent. The total MNPs in surface water without adsorbent were 2.16, 0.07, 0.10, and 0.03 µg/L for PVC, SBR, PC, and N6, respectively. Meanwhile, the water sample with adsorbent presented 12.93, 1.37, 0.87, 0.01, and 0.10 µg/L. Therefore, the adsorbent can improve the collecting MNPs through adsorption process which increase the performance of MNPs analysis.

Keywords: microplastics; nanoplastics; surface water; SBA-15; PY-GC-MS

Dr. Chanatip Samart received a Ph.D. in Chemical Engineering (2006) from Kasetsart University. He is currently Associate Professor at Thammasat University, where he leads a research group in biorefinery and catalyst development. His work focuses on transforming biomass into fuels and valuable chemicals, including ultrasonic-assisted biodiesel, catalytic pyrolysis, and electrochemical biomass upgrading

TU-Frontier Lab-JEOL joint session Contaminants of Emerging Concern: PFAS & Microplastics (SB-I-006)

Determination of microplastics particles in natural waters by pyrolysis-GCMS

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Microplastics (MPs) is classified as an emerging contaminant, which has been receiving greater attention in the recent past. Studies have found microplastics in the environment (air, soil and water) as well as in food. It is evident that microplastics is making their way into our bodies too. Studies have found microplastics in human blood, urine etc. However, its impact on human health is not fully understood. Bioaccumulation of microplastics food chain is of great concern due to which even small concentration today can pose a threat in the future. Research efforts are ongoing to improve our understanding on microplastics detection, distribution and toxicological effects which are essential for federal agencies and policy makers to understand the issue and implement some measures.

Accurate identification and quantification are primary steps in understanding and mitigating microplastics impacts. From recent research reports, it is evident that mass-based analysis should be an integral part of Microplastics analysis. In this work, we present simple workflow for mass determination of microplastics from natural waters. A small volume of water samples is filtered through glass fiber filter media, and the filter media is directly analyzed by Pyrolysis-GCMS for identification and quantification. Analytical method details and method performance data will be presented and discussed. This work will emphasize QA/QC protocol to increase confidence levels in analysis. Finally, we will present some real-world samples data to demonstrate the method suitability for environmental monitoring campaigns.

Keywords: environment; pollution; microplastics; pyrolysis-GCMS

Dr. Sathrugnan Karthikeyan has received PhD in Analytical Chemistry from Cochin University of Science and Technology, India and did postdoctoral research at Texas Tech University, USA and AIST, Japan before moving to Singapore. He has been working in Singapore for more than 20 years in academia and industry at different capacities. His research interests are analytical chemistry, environmental science, food and environmental safety, materials characterization and pyrolysis. He is currently working as Regional Technical Manager at Frontier Laboratories, Japan.

Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-I-003)

Homogeneous catalysis by coordination complexes of mismatched donor-acceptor pairs

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Ligand design plays an important role in exploratory research on contemporary industry, coordination chemistry, and homogeneous catalysis. This presentation describes the origin and accumulative development of PNP amido phosphine complexes and their isoelectronic analogues constructed with an ortho-phenylene backbone. With the incorporation of both soft and hard donors in the hybrid ligands, these complexes are inherently characteristic of having mismatched donor-acceptor pairs. Complexes containing ligands having meridional and facial coordination modes are exemplified with their physical preferences and chemical activities in bond-forming and bond-breaking transformations. The effects of P-substituents and ligand backbones of these complexes on reaction and structural chemistry are presented. Emphasized are the developments of these complexes in homogeneous catalysis.

Keywords: homogeneous catalysis; mismatched donor-acceptor pairs; hard and soft acids and bases

Lan-Chang Liang is a Distinguished Professor of Chemistry at National Sun Yat-sen University and joint Professor at Kaohsiung Medical University. He earned his PhD at MIT under Nobel Laureate Richard R. Schrock, focusing on early transition metal chemistry. After postdoctoral work at Stanford, his research at NSYSU centers on mismatched coordination compounds for chemical bond activation and catalytic functionalization. His achievements include the Thieme Chemistry Journals Award, recognition as a top international inorganic chemist under 40, and the Chemical Society of Japan's Distinguished Lectureship Award.

Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-I-006)

Approaches to the design of oxygen-tolerant electrocatalysts for hydrogen evolution reaction

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The development of efficient electrocatalysts for the hydrogen evolution reaction (HER) is pivotal to advancing a sustainable hydrogen economy. Over the past decade, tremendous progress in HER electrocatalysts has been achieved. Nevertheless, most HER electrocatalysts remain unstable in the presence of molecular oxygen, which impedes practical applications. This instability arises from the greater tendency of the O_2 reduction reaction (ORR) to generate reactive oxygen species, such as superoxide or hydrogen peroxide, compared to HER. In this talk, I will highlight how the incorporation of a secondary coordination sphere within a molecular cobalt complex not only facilitates HER but also enhances its oxygen tolerance. In addition, this SCS site acts as a proton relay centre to modulate the proton transfer route (i.e., intramolecular and intermolecular proton transfer), thereby affecting the oxygen tolerance of the cobalt complex.

Keywords: oxygen-tolerance; electrocatalysts; hydrogen evolution reaction; oxygen reduction reaction

Vincent Wang grew up in Taiwan and obtained his BS and MS degrees from National Taiwan University and his DPhil degree from the University of Oxford. He began his independent career in 2021 as an assistant professor. His research encompasses the design and mechanistic elucidation of photocatalysts and electrocatalysts involved in energy conversion processes. For more information, please visit www.teamvw.org.

Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-I-008)

Durable anode electrocatalysts through acidic redox-assisted deposition for seawater electrolysis

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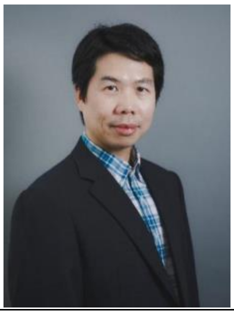
Direct seawater electrolysis presents a substantial challenge to the advancement of the green hydrogen industry, primarily due to two critical issues: the corrosive nature of seawater and the release of toxic chlorine gas during the process. These challenges have hindered the development of efficient, long-lasting seawater electrolyzers, which are essential for large-scale hydrogen production.

Our team has developed a novel technique called redox-assisted deposition (ARD), which we will demonstrate as a method for producing multi-metal oxide materials. These materials exhibit high elemental homogeneity, improved conductivity, and enhanced stability under harsh operational conditions. ARD deposition has proven to offer strong adhesion on various substrate surfaces, ensuring the durability needed for extended operation in alkaline seawater electrolyzers. Notably, this coating provides significant protection to the gas diffusion layer, which plays a vital role in the system's performance.

In our experiments, ARD-coated electrodes were able to stably support seawater electrolysis for 150 hours at a current density of 100 mA/cm^2 and a voltage of 1.9 V. Without the protective ARD layer, the metal components succumbed to corrosion in as little as 1 to 2 hours. Moreover, we employed in-situ mass spectrometry to monitor chlorine gas production, and no chlorine gas was detected throughout the experiment. This finding underscores the ability of ARD deposition to mitigate chlorine emission.

The ARD technique holds significant promise as a solution to the current limitations of direct seawater electrolysis. The chemical principles, synthesis process, and underlying mechanisms of ARD will be discussed in detail, providing insight into how this method addresses the key technical challenges of corrosion and chlorine emission, and paving the way for more sustainable hydrogen production from seawater.

Keywords: seawater; alkaline water splitting; anion exchange membrane; bilayer; adhesion



Distinguished Professor Chun-Hu Chen (born in 1978) of National Sun Yat-sen University (NSYSU) is a leading expert in materials chemistry, specializing in graphene-metal oxide nanocomposites and clean energy solutions. He holds a Ph.D. from the University of Connecticut (2010) and focuses on hydrogen production, particularly using water-splitting technologies. His work has significantly reduced the cost of green hydrogen production, advancing sustainable energy storage.

Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-I-009)

Electrolyte additives for enhanced performance in lithium-ion batteries

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The development of high-voltage lithium-ion batteries is limited by electrolyte instability and the formation of unstable cathode–electrolyte interphase (CEI) layers. This presentation introduces two types of molecularly engineered electrolyte additives—fluorinated boronates and (pentafluorophenyl)diphenylphosphine (PFPDPP)—that improve interfacial stability on $LiNi_{0.5}Mn_{1.5}O_4$ cathodes. Density functional theory and electrochemical measurements reveal that these additives decompose preferentially to form protective CEI films prior to electrolyte oxidation. Advanced characterizations, including scanning electron microscopy, transmission electron microscopy, X-ray photoelectron spectroscopy, and impedance spectroscopy, show that the additives yield thinner, denser, and less resistive CEI layers while effectively suppressing LiF formation. These interfacial improvements lead to significant enhancements in cycle life, rate performance, and thermal stability. The results offer new insight into structure–function relationships for additive design and present a rational strategy for next-generation high-voltage lithium-ion batteries.

Keywords: high voltage; electrolytes; additives; $LiNi_{0.5}Mn_{1.5}O_4$; cathodes

He earned his Ph.D. from National Tsing Hua University in 2001. After working at the Industrial Technology Research Institute and completing postdoctoral research at the University of Illinois at Urbana-Champaign, he joined National Sun Yat-sen University in 2008. He became Professor and Chair (2018–2024) and now serves as Dean. His research focuses on lithium-ion, organic, and flow batteries. He has received numerous honors, including Distinguished Junior Research Professor (2012–2015), Outstanding Industry-University Cooperative Research Award (2018–2023), and Outstanding Research Awards (2018–2021, 2023, 2024).

IMS-CU Bilateral Symposium for Driving Forward Frontier Research (SD-I-001)

Rational engineering of high performance artificial molecular motors

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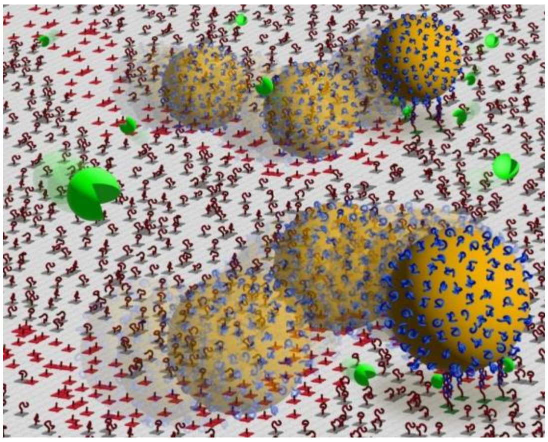
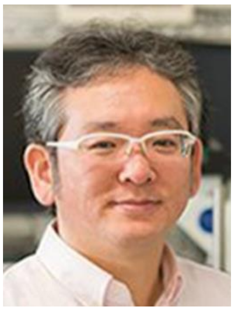
Engineering artificial molecular motors with high performances is an important challenge to implement them in biological and abiotic systems. DNA is not only a fundamental molecule of living organisms but also a versatile building block used to engineer a variety of artificial molecular motors. DNA-nanoparticle motor is one of the fastest nanoscale artificial motors and moves on RNA-coated surface driven by RNase H. However, its speed is much lower than those of natural motor proteins. Here we resolve its elementary processes of motion (pauses and steps) and reveal long pauses caused by slow RNase H binding are the bottleneck. As RNase H concentration increases, pause lengths shorten from ~70 s to ~0.2 s, while step sizes are constant (~20 nm). At high RNase H concentration, speed reaches ~100 nm s^{-1}, however, run-length and unidirectionality largely decrease. A newly-developed geometry-based kinetic simulation reveals elementary chemical reaction processes which cause pauses and steps, and trade-off mechanism between speed and other performances. A rationally-engineered motor with 3.8-times larger DNA/RNA hybridization rate simultaneously achieves 30 nm s^{-1} speed and 3 μm run-length comparable to motor proteins, and high unidirectionality. In future, we develop artificial molecular motors that surpass motor proteins, and establish methods of motion-based molecular computations and biomarker detections.

Keywords: molecular motors; DNA nanotechnology; single-particle tracking; kinetic simulation





Ryota Iino is a distinguished biophysicist who earned his doctoral degree in 2003 from and has built a prolific academic career across top Japanese institutions. He currently leads research at IMS on single-molecule observation of biological molecular machines, capturing their dynamic behavior with cutting-edge imaging techniques.

Chirality-induced spin selectivity in chiral solids

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Chirality-Induced Spin Selectivity (CISS) is attracting recent attention as a new source of spin polarized current. It also provides unique methods for enantio-separation, enantio-selective electrochemical reactions, and efficient water oxidation. The mechanism of CISS effect is, however, yet to be clarified, as the effect is much larger than expected one estimated with small spin-orbit coupling for organic molecules. In a hypothetical consideration, it is proposed that an enhancement of spin polarization is associated with anti-parallel spin pair at two opposite ends of a chiral molecule. It is interesting to note that such an anti-parallel spin pair is a time-reversal (*T*) odd state, while the chiral molecular structure is *T*-even. We think symmetry conversion from *T*-even to *T*-odd quantities gives an essential clue to understand CISS effect that can generate huge spin polarization in a non-equilibrium condition.We have made such a symmetrical consideration based on multipole basis and found that a *T*-odd chirality can e merge from an accumulation of spin current at reservoirs. In a chiral metal, we have confirmed that the CISS effect appears as spin polarization rather than spin filtering. In addition, we have shown that chiral organic superconductors can exhibit spin accumulation at two opposite crystal edges whose directions are anti-parallel to one another. This can be regarded as a macroscopic-size emulation of chiral molecules that has *T*-odd spin pairs at their opposite ends. A connection to falsely chiral influence will be also discussed.

Keywords: chiral materials; superconductor; spintronics; CISS effect

Hiroshi Yamamoto received his D.Sc. in solid state chemistry at the University of Tokyo in 1998. He spent one year as an assistant professor at the Department of Physics, Gakushuin University, and 13 years as a research scientist at RIKEN. Since 2012, he has served as a full professor at the Institute for Molecular Science, National Institutes of Natural Sciences in Japan. His research interests focus on organic electronics and spintronics based on novel operation mechanisms. Organic superconductor transistors and spintronic devices based on chirality are two major current topics in his study.

IMS-CU Bilateral Symposium for Driving Forward Frontier Research (SD-I-003)

One day about 2.2 billion years ago, cyanobacteria anticipated the timing of the next sunrise

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We can see various rhythmic phenomena around us. Biological phenomena that oscillate in a cycle of approximately 24 hours, the same cycle as the earth's rotation, are called circadian clocks. The circadian clocks have three physiological properties: self-sustained oscillation with the circadian period, temperature insensitivity (compensation) of the cycle length, and entrainment to environmental cycles. There is no doubt that organisms have acquired clock functions over the course of their long evolution, but the details are not well understood. We have been studying the evolution of the circadian clock in cyanobacteria by taking advantage of the fact that it can be reconstituted in a test tube. In this presentation, I would like to discuss our hypothesis on the past evolution of the circadian clock in cyanobacteria and the possibility of its further evolution in the future.

Keywords: cyanobacteria; circadian clock; evolution

Shuji Akiyama received his Ph. D. in chemistry of molecular engineering at Kyoto University in 2002. After postdoctoral research fellows at JSPS , RIKEN, and JST, he was appointed as a junior associate professor of Nagoya University in 2008 and then as an associate professor in 2011. Since 2012, he serves as a full professor at Institute for Molecular Science, National Institutes of Natural Sciences in Japan. His research interests focus on chemistry of biological rhythms and dynamics, especially circadian clock system in cyanobacteria.

IMS-CU Bilateral Symposium for Driving Forward Frontier Research (SD-I-004)

Molecular dynamics simulation of protein aggregation

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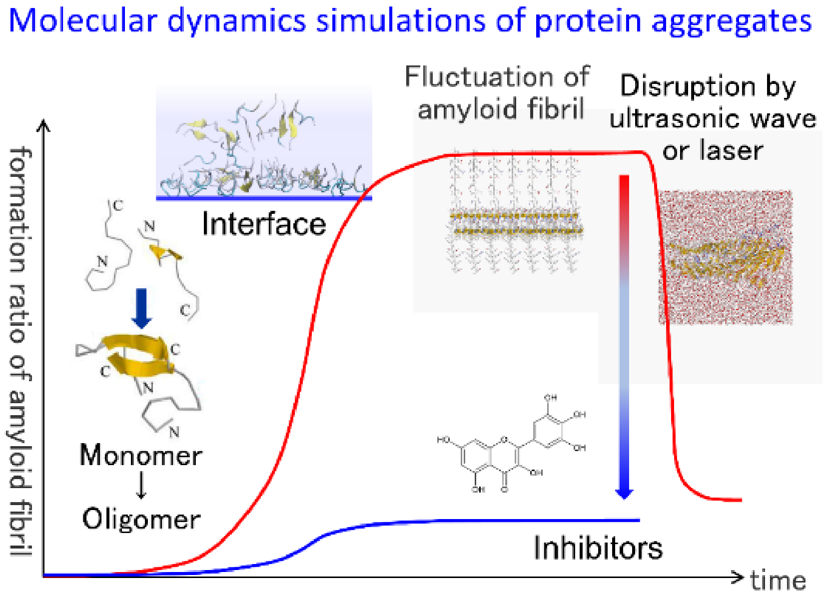
Protein aggregates sometimes cause several diseases such as Alzheimer’s disease and Huntington’s disease. Aggregates of amyloid-β (Aβ) peptides cause Alzheimer’s disease and those of poly-glutamine cause Huntington’s disease. We have studied several topics on these protein aggregates by molecular dynamics (MD) simulation. In my talk, several MD simulation studies are introduced, such as the aggregation of Aβ peptides in bulk solution [ACS Chem. Neurosci. 13 (2022) 3139], at the interface [J. Chem. Phys. 151 (2020) 095101], and under the shear [J. Chem. Theory Comput. 20 (2024) 10199–10208]. We will discuss the mechanisms of these aggregation processes.

Keywords: molecular dynamics simulation; protein aggregate; amyloid



Hisashi Okumura earned his Ph.D. in Physics from Keio University (2002) and progressed through roles at UTokyo, IMS, Nagoya University, Rutgers, and SOKENDAI. Since May 2009, he has served as Associate Professor at both IMS and SOKENDAI, taking on his current role in 2018 at the Exploratory Research Center on Life and Living Systems. His research focuses on advanced MD simulations of biomolecules, with significant contributions to understanding protein aggregation and amyloid disruption. In 2014, he received the Molecular Simulation Society of Japan’s Academic Award for his methodological innovations.

IMS-CU Bilateral Symposium for Driving Forward Frontier Research (SD-I-005)

Microwave-assisted, shape-controlled synthesis of nanoparticles: The case of iron oxide nanocubes

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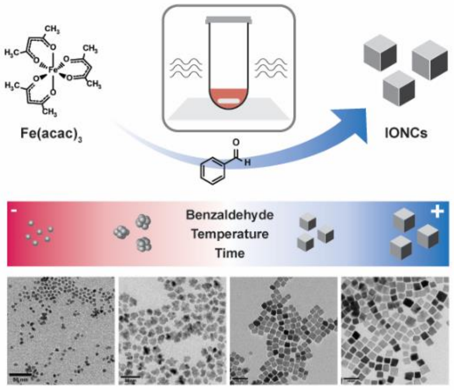
Controlling shape is a topic of interest in the field of nanoparticle synthesis. Nanoparticles with certain shapes exhibit unique and enhanced properties. Iron oxide nanocubes (IONCs) are effective agents for cancer magnetic hyperthermia (MH) due to their shape anisotropy. Conventional synthesis techniques for IONCs require long reaction times and suffer from poor reproducibility. Therefore, there is a need for faster and more reproducible synthesis techniques. In this work, we developed a rapid microwave-assisted synthesis method for IONCs. Using this method, IONCs were successfully synthesized in less than 30 minutes with high reproducibility. The size of the IONCs can be tuned between 13 and 30 nm by adjusting synthesis parameters, including reaction time, temperature, and the amount of benzaldehyde which serves as the shape-directing agent. This synthesis method gave a high iron conversion yield of up to 80%. The obtained IONCs exhibited size-dependent heating efficiency with high specific absorption rate values of up to 400 $W \cdot g^{-1}$ under clinical alternating magnetic field conditions. Thus, the method developed in this work provides a fast and reproducible synthesis of IONCs with notable MH properties and potential for large-scale production in the future.

Keywords: iron oxide nanocube; magnetic hyperthermia; microwave-assisted synthesis; nanomaterials



Wid Mekseriwattana received his Ph.D. in Materials Science and Engineering in 2022 from Mahidol University, Thailand. He then worked as a postdoctoral researcher at the Italian Institute of Technology, focusing on nanoparticles for biomedical applications. He is currently a lecturer in chemistry at Chulalongkorn University. His research interests lie in the synthesis of inorganic and hybrid nanomaterials and their interactions with biological systems. Particularly for applying the intrinsic properties of materials in biomedical and environmental fields.

IMS-CU Bilateral Symposium for Driving Forward Frontier Research (SD-I-006)

Enhancing the catalytic efficiency of MOFs for cellulose hydrolysis via postsynthetic modification with chlorosulfonic acid

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The improper handling of agricultural biomass waste, particularly open burning, is a significant contributor to environmental issues, including air pollution and climate change. A sustainable approach to address this issue is the conversion of biomass waste, which contains 40-45% cellulose, to valuable chemicals via hydrolysis. This process produces glucose, a key intermediate for valuable chemicals such as 5-HMF, sorbitol, ethanol, and levulinic acid. However, the conventional method, which utilizes mineral acids, is unsustainable since it is costly and generates hazardous waste. This study explores the alternative method based on NU-1000, a pyrene-based MOF. We focused on enhancing its catalytic efficiency for cellulose hydrolysis through postsynthetic modification using chlorosulfonic acid. The postsynthetic modification process significantly enhances both percent conversion and selectivity for the hydrolysis of cellobiose and cellulose into glucose. Our investigation of the MOF structure after postsynthetic modification via spectroscopic and crystallographic analyses revealed the reason behind the enhanced catalytic activity of the MOF. In this presentation, I will discuss the results from structural investigation as well as the potential of the MOF as a catalyst for cellulose hydrolysis.

Keywords: MOF; postsynthetic modification; cellulose hydrolysis; NU-1000; biomass waste

Preecha Kittikhunnatham earned his Ph.D. in Physical Chemistry from the University of South Carolina, where he also completed postdoctoral training in Inorganic Chemistry. He is currently serving as a lecturer at Chulalongkorn University. His research focuses on the synthesis of functional high-surface-area materials, such as metal–organic frameworks and nanomaterials, for applications in areas including heterogeneous catalysis.

IMS-CU Bilateral Symposium for Driving Forward Frontier Research (SD-I-007)

Revisiting the desulfurization process via photochemical or electrochemical routes: A mild and green approach to heterocycle synthesis

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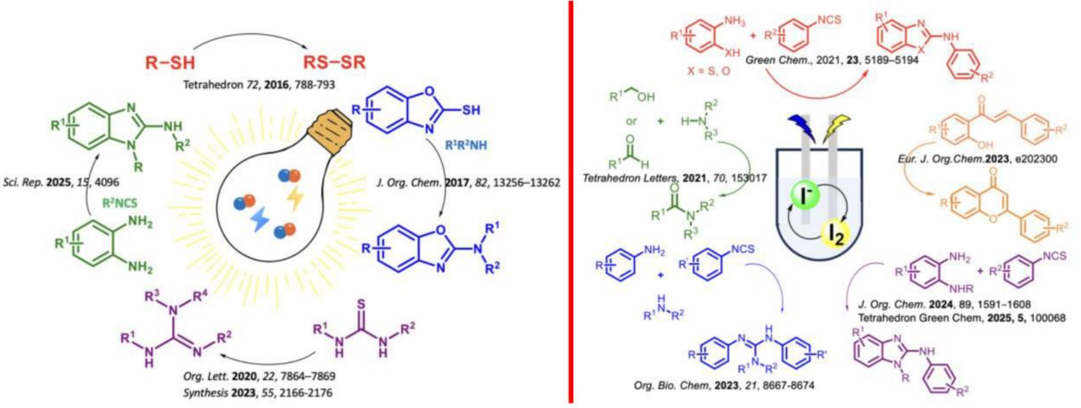
As a young researcher, I had the privilege to join the JSPS (Japan Society for the Promotion of Science) program in 2009 at the Institute for Molecular Science (IMS), Okazaki, Japan. During this 40-day collaboration with Prof. Uozumi, I worked on heterogeneous catalysis for asymmetric synthesis in water (WOW). This experience profoundly shaped my perspective and continues to influence the direction of my research today.While I never set out to reinvent the wheel, my goal since then has been to help transform traditional organic synthesis often reliant on stoichiometric and hazardous reagents into milder, safer, and more sustainable processes that retain both effectiveness and economic viability.

In this work, I present two distinct green approaches to desulfurization: (1) a photochemical method and (2) an electrochemical method. Each independently enables efficient synthesis of valuable heterocycles, including amides, 2-aminobenzoxazoles, chalcones, guanidines, and aminobenzimidazoles, under environmentally friendly conditions.

Keywords: electrochemical oxidation; desulfurization; iodide mediator; catalytic amount; photo catalyst



Sumrit Wacharasindhu, Chulalongkorn University (B.Sc. 2000), University of Missouri-Columbia (Ph.D. 2005, Prof. Michael Harmata), Wyeth Pharmaceuticals (now Pfizer) (Postdoc, 2005–2007), Lecturer (Chulalongkorn University, (2007-2010), Assistant professor (2010–2015), Associate professor (2015–2020), Professsor (2020–present) Research field: Green synthetic methodology development and sensor based on conjugated polymers

Cinnamon bark oil-based gelatin-chitosan composite films for active food packaging application

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Cinnamon bark oil (CBO) is well recognized for its strong antimicrobial properties. Encapsulation of the oil within a polymer matrix results in microcapsules (MCs) which will mitigate the high volatility of essential oils and provide protection against oxidation, heat and radiation, ease of handling, prolonged bioavailability. CBO was encapsulated in polymeric chitosan (CS) matrix and gelatin-chitosan films were prepared incorporating these CBO-CS-MCs. Antibacterial activity of the CBO-Gelatin-CS films were tested against three foodborne pathogens: *Escherichia coli*, *Bacillus subtilis* and *Salmonella typhi* by measuring the optical density (OD) of the cultures at 560 nm. Empty CS-MCs (without oil) incorporated gelatin-CS films were used as the negative control and free CBO incorporated Gelatin-CS films were also used as a treatment. All treatments were triplicated. The oil encapsulation efficiency and the oil load in MCs were 83% and 16% respectively. CBO-CS-MCs showed 100% inhibition of all three bacterial strains at 20 mg of oil (MID) in MCs. Films prepared incorporating free CBO and CBO-CS-MCs at MID, showed a good inhibition of bacterial strains. Nevertheless, the inhibitory activity of free CBO containing films gradually decreased with time. CBO-Gelatin-CS films provide potent antimicrobial films for active food packaging applications.

Keywords: chitosan; cinnamon bark oil; microcapsules; antibacterial films

Toxic metals and their availability to paddy (*Oryza sativa*) plants via inorganic fertilizers: A study in a CKDu hotspot in the north central province in Sri Lanka

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Agriculture has been dominated by paddy in Sri Lanka's dry zone where the chronic kidney disease of unknown etiology (CKDu) has prevailed over decades. Inorganic fertilizers which are blended with a range of trace metals are severely used in paddy cultivation. The objective of this study is to determine the toxic metals and their availability to paddy (*Oryza sativa*) plants via soil fertilized with inorganic fertilizers in a CKDu hotspot in the north central province in Sri Lanka and to explore the relationships between CKDu prevalence and trace metals containing fertilizers. The average concentrations of toxic metals in the agricultural soils (before cultivation and after harvesting) carried a sequence of Mn > Cr > Zn > Cu > Pb > As > Cd. Concentrations of Cd, Pb, Cu and Zn of paddy soil after harvesting were significantly higher than those of before cultivation. Experimental results show that triple superphosphate (TSP) contains the highest concentrations of Cd, Pb, Cr, Mn and Cu as impurities and urea fertilizer has the highest contents in As and Zn. The results further describe the risk of accumulating nephrotoxic heavy metals in residents of the sampling area. Therefore, there can be a direct relationship between the consumption of rice containing nephrotoxic heavy metals and the CKDu prevalence in the sampling area.

Keywords: CKDu; inorganic fertilizers; nephrotoxicity; toxic metals; *Oryza sativa*

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-I-013)

Absorption of selected pesticide residues during cooking by *Murraya koenigii*

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Curry leaves, *Murraya koenigii* is a fascinating house plant grown in Asia. The leaves of *M. koenigii* are added to Sri Lankan cuisine due to their aroma and health benefits. However, the growing trend of using chemical pesticides in Sri Lanka results in vegetables contaminated with pesticide residues. Although various methods have been studied for removing pesticide residues on fresh vegetables, none effectively removes pesticide residues 100%. Therefore, pesticides can still remain on vegetables even after washing. Since the leaves of *M. koenigii* are used in cooking vegetables, pesticides remaining in vegetables may be absorbed by curry leaves during cooking. In the current study, we aim to understand the effectiveness of curry leaves as a scavenger of toxic pesticide residues during cooking and to increase the awareness of the fate of the pesticides during cooking.

The analysis was carried out by using a HPLC-UV with QuEChERS. Our results showed that the *M. koenigii* leaves can absorb the pesticides from the vegetables contaminated with pesticides during cooking. With the absorption of pesticides, a considerable decrement of major carotenoid content was observed, while the carotenoid profile remained unaltered. Therefore, *M. koenigii* leaves are a scavenger of pesticides when cooking pesticide-contaminated vegetables.

Keywords: pesticides; HPLC; *Murraya koenigii*; carotenoid; QuEChERS

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-I-014)

Exploring the therapeutic potential of *Dialium ovoideum* Thwaites

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Dialium ovoideum Thwaites, an endemic plant of Sri Lanka, has traditionally been valued for its medicinal properties. This study investigated the bioactive compounds and biological activities of various parts of the plant, including leaves, bark, pulp, peel, and seeds. Significant biological activities, such as antioxidant, anti-inflammatory, anti-tyrosinase, antimicrobial, and antiglycation effects, were demonstrated. Spectroscopic assays, including the Folin-Ciocalteu method and aluminum chloride assay, were used to determine total phenolic content (TPC) and total flavonoid content (TFC). Antioxidant activity was assessed using DPPH radical scavenging and FRAP assays, while anti-inflammatory, anti-tyrosinase, antimicrobial, and antiglycation activities were evaluated using the human red blood cell (HRBC) stabilization assay, modified DOPA-chrome method, agar-well diffusion method, and bovine serum albumin assay, respectively. The bark exhibited the highest levels of phenolic and flavonoid compounds and showed promising antioxidant and anti-inflammatory activities. Consequently, ethanol bark extract was selected for compound isolation and the development of value-added products, including a topical anti-inflammatory herbal cream with excellent potential for skincare applications. By emphasizing the remarkable therapeutic potential of *Dialium ovoideum*, this research highlights the importance of biodiversity conservation and the role of endemic plants in advancing natural product research and cosmeceutical innovations.

Keywords: bioactive compounds; biological activities; bark extract; *Dialium ovoideum* thwaites; herbal cream

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-I-015)

Appraisal of toxic metal contamination of agricultural soil and food in upcountry and CKDu-endemic lowland regions of Sri Lanka

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Long-term consumption of foods contaminated with toxic metals may increase the risk of noncommunicable diseases, including chronic kidney disease of uncertain origin (CKDu). This study aims to evaluate the accumulation of heavy metals and metalloids in agricultural soil and crops, and inland fish from selected CKDu-endemic and non-endemic areas, compare contamination levels, and assess patterns of metal transfer. The findings from studies conducted in upcountry areas (Shanthipura Division, Nuwara Eliya; reference site) indicate that Pb, Cd, Ni, and Cr levels in soil remain within permissible limits (MPLs). Vegetable samples contained lower heavy metal levels than WHO limits, with Ni being undetectable. The analysis of Cr, Cd, As, and Ni concentrations on food samples from the CKDu-endemic Mihinthalaya Division, Anuradhapura, revealed that these metals remained within MPLs. However, Pb levels exceeded MPLs in rice (*Oryza sativa*), leafy vegetables, and inland fish (*Etroplus suratensis*). Notably, the average concentrations of metals and metalloids in agricultural soil and crops were higher in the endemic area than the reference. Moreover, hierarchical analysis suggested a common source of Pb accumulation in soil, and food samples of the endemic area, while principal component analysis (PCA) and hierarchical clustering revealed a strong correlation between As and Cd, indicating a potential shared origin.

Keywords: bioaccumulation; CKDu; soil; toxic metals

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-I-016)

Biochar surface functionality as affected by acid-base modifications: FTIR-based principal component analysis

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Biochar (BC) is a carbonaceous, porous material with unique surface properties, extensively studied for its potential in environmental remediation and soil enhancement. Modification processes, including mineral acid and base treatments, improve its physicochemical properties for targeted applications by enhancing surface functionality, structural integrity, and surface area. Key characteristics of BC, such as surface functionality, morphology, and aromaticity, govern its adsorption capacity, with surface functionality being particularly influential. Although the relationship between feedstock type and physicochemical traits is well-studied, the effects of surface functionality modifications based on feedstock type remain underexplored. This study addresses the gap by applying principal component analysis (PCA) to FTIR data to systematically assess how modifications affect BC surface functionality across varied feedstocks. Both raw and modified BC, derived from three lignocellulosic and three non-lignocellulosic feedstocks, were subjected to mineral acid and alkaline treatments. PCA revealed distinct clusters, indicating modifications influenced physicochemical properties in a feedstock-dependent manner, with clear differentiation between lignocellulosic and non-lignocellulosic biomasses. The observed clustering demonstrated a statistical correlation driven by modification types. The developed model offers deeper insight into how surface functionality is altered by specific modifications, a critical factor governing BC's adsorption behavior and enhancing its applicability in environmental solutions.

Keywords: biochar; surface functionality; feedstock; principal component analysis

Sustainable Chemistry for Agricultural Residue Valorization (SG-I-001)

Furfural production from raw biomass using formic acid as a solvent and catalyst: Optimization and extraction methods

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This study establishes a proof of concept for using formic acid as both a fractionation solvent and a catalyst in the production of furfural from raw biomass. The operating parameters were first optimized in a batch system using synthetic solutions containing xylose (10-30 g/L) with 10 wt% formic acid. The optimal conditions were determined to be 170 °C, 40 min, and an initial xylose concentration of 10 g/L, resulting in a furfural yield of 58%. Subsequently, these conditions were applied to biomass-derived hydrolysates, free of cellulose and lignin, obtained via formic acid hydrolysis of fir wood and oil palm empty fruit bunches (OPEFB), resulting in furfural yields of 55% and 70%, respectively. Two extraction methods were used to extract furfural from the reaction medium: steam stripping in a semi-batch system with a steam flow rate of 3.5 mL/min, and a biphasic solvent system with a 1:3 (v/v) water-cyclopentyl methyl ether ratio. Both methods significantly increased furfural yield, achieving a separation efficiency exceeding 90%. Furfural yield from fir wood increased to 72% in the semi-batch system and 76% in the biphasic system. Similarly, OPEFB yielded 79% in the semi-batch system and 83% in the biphasic system. These results demonstrate the effectiveness of this approach in achieving high furfural yields directly from raw biomass, supporting its potential application in integrated biorefinery systems.

Keywords: biomass; formic acid; furfural; extraction methods

Dr. Kritsana Namhaed, born in 1995, received a scholarship from the Ministry of Higher Education, Science, Research and Innovation of Thailand to pursue his studies in France from 2015 to 2024. He earned his Ph.D. in Process and Environmental Engineering from the Institut National Polytechnique of Toulouse. Currently, he serves as a lecturer in the Department of Chemical Engineering, Faculty of Engineering and Industrial Technology, Silpakorn University, Nakhon Pathom, Thailand. His research focuses on green process engineering and renewable energy technologies, with particular emphasis on biomass valorization, catalysis, and separation processes.

Sustainable Chemistry for Agricultural Residue Valorization (SG-I-002)

Potential sources for valorization of agricultural wastes from economic crops in the lower central region of Thailand

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In this talk, we discuss the valorization of agricultural wastes from economic crops in lower central region of Thailand including Nakhon Pathom, Ratchaburi and Kanchanaburi. Agricultural wastes from coconuts, bananas, mangoes, and cocoas are great sources of biomass. Valorization of the biomass can lead to valuable platform chemicals. Mango and banana peels contain high level of sugars and cellulose. Hydrolysis of cellulose to glucose and fructose, isomerization of glucose to fructose and dehydration of fructose gives 5-hydroxymethylfurfural (5-HMF), a versatile and valuable platform chemical. The woody husks of coconut and cocoa contain lignocellulose. Pretreatment of lignocellulose gives lignin, cellulose and hemicellulose. Lignin can be converted to aromatic platform chemicals by depolymerization giving phenols, *p*-coumaryl alcohol and vanillin, etc. We have initiated a joint research project among researchers at the Faculty of Science, Silpakorn University, applying physical and chemical techniques for valorization of these biomasses. Preliminarily, a process for production of 5-HMF from dried fruit peels has been established. The project is carried out in collaboration with local agricultural community enterprises and fruit processing companies who provide agricultural wastes. These include banana peels from solar-powered dried banana, mango peels from mango paste and pickled mango producers. Local companies that process agricultural products such as coconut water and cocoa powder provide coconut and cocoa husks. The objectives of this study are to reduce cost and adverse environmental impact of agricultural waste disposal, enhance the value of agricultural crops and encourage zero-waste agricultural practice for more sustainable future.

Keywords: agricultural waste; economic crops; valorization; sources

Punlop Kuntiyong (b. 1975), พัลลภ คันธิยงค์

Education: PhD. (Chemistry), Oregon State University, Oregon, USA (2004). Current Position: Associate Professor (Organic Chemistry), Department of Chemistry, Faculty of Science, Silpakorn University, Nakhon Pathom, Thailand.

Research Interests: Asymmetric synthesis of biologically active alkaloids. Awards: ACP Lectureship awards 2014 to Japan and Taiwan, ACP Lectureship awards 2019 to Korea and China.

Lignin as a biofunctional material: Multidisciplinary approaches in lignin valorization

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Lignin, a complex aromatic polymer found in biomass, presents opportunities in various applications, including sustainable biorefineries and advanced materials or drug initiators for medical use. Experimental studies have provided key insights into its structure, properties, and potential applications. However, bridging the gap between experimental findings and comprehensive understanding often requires support from computational chemistry methods such as quantum mechanics (QM), molecular dynamics (MD) simulations, cheminformatics, and hybrid computational approaches. These techniques are employed to study chemical reactions involving lignin by predicting thermodynamic profiles and mechanistic pathways, thereby facilitating the design of effective lignin valorization strategies.

Lignin also shows great potential in the health sciences and pharmaceutical industries. Its structural diversity and inherent bioactivity offer possibilities for developing drug delivery systems, biocompatible scaffolds, and other biomedical applications. Lignin-based materials exhibit antioxidant, antimicrobial, and anti-inflammatory properties, making them promising candidates for wound healing, tissue engineering, and medical device coatings. Although significant progress has been made in these areas, further interdisciplinary research is needed to fully unlock the potential of lignin in the areas.

In my talk, this interdisciplinary gap will be addressed in order to deliver some ideas on how to maximize lignin potential across biomedical and pharmaceutical sectors and advancing its role in the transition to sustainable, bio-based healthcare solutions.

Keywords: Lignin valorization; computational chemistry; biomedical applications

Pemikar Srifa, Ph.D. (b. 1986), is a lecturer at Faculty of Medicine, Prince of Songkla University. She received her Ph.D. in Organic Chemistry form the Department of Organic Chemistry at Stockholm University, Sweden. Her research focuses on the design and development of materials used for medical purposes, bioactive molecules, and drugs. She also conducts in silico studies of interactions between pathogen proteins or biomarkers and their target biomolecules for personalized medicine development.

Biomass-to-coating innovation: Eco-friendly solutions from palm residue valorization

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Oil palm is a major economic crop in Thailand and the third-largest source of agricultural residue, producing up to 38 tons of biomass per hectare. Upcycling empty fruit bunches (EFB) into value-added products offers a sustainable way to increase farmer income and national GDP. This study presents the development of eco-wood coatings derived from EFB. The process involves the fractionation of EFB lignocellulose into lignin, cellulose, and hemicellulose. Lignin is chemically modified to improve solubility, while cellulose and hemicellulose are converted into bio-based solvents using green catalytic methods. These components are formulated into eco-wood coatings that exhibit low VOC emissions and non-toxic properties. The resulting product meets both Thai: TIS 1513-2563 and European: EN 71-3:2019 safety standards for wood coatings. The innovation has been validated from laboratory to bench scale, demonstrating its scalability and potential for commercialization. This development aligns with the Bio-Circular-Green (BCG) economy model and supports the UN Sustainable Development Goals (SDGs) by promoting waste valorization, green chemistry, and safer consumer products.

Keywords: empty fruit bunch (EFB); biomass separation; bio-based solvents; lignin modification; eco-wood coating

Assistant Professor Dr. Duangamol Tungasmita (Nuntasri) is a faculty member at the Department of Chemistry, Faculty of Science, Chulalongkorn University. She obtained a Ph.D. from Yokohama National University, Japan, in 2003. Her research focus on green chemistry, material synthesis and catalytic application. She has been active in the Asian Network of Green Chemistry since 2012 and received the Western Digital Innovative Award in 2014. She has published 42 papers, filed 18 patents, and has an h-index of 16.

ORAL ABSTRACTS

Analytical Chemistry (AC-O-007)

Coupling gas chromatography–mass spectrometry with spray-assisted liquid phase microextraction for determining flibanserin in synthetic urine samples

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The first medication approved to treat hypoactive sexual desire disorder (HSSD) in premenopausal women is flibanserin [*Microchem. J.* **2021**, *164*, 105960]. Flibanserin has pharmacological effects by increasing extracellular concentrations of norepinephrine and dopamine while simultaneously suppressing serotonin [*Microchem. J.* **2021**, *167*, 106281]. After the oral administration of a single 100-mg dose of flibanserin, the mean terminal half-life was approximately 10 hours, with 44% removed in urine [*Molecules* **2020**, *25*, 4932]. This study presents highly efficient recovery studies in synthetic urine samples through combining spray-assisted liquid phase microextraction (SA-LPME) with gas chromatography-mass spectrometry (GC-MS) for the accurate and precise quantification of flibanserin. The parameters of SA-LPME, which include spray cycle, extraction solvent type, mixing type, and period, were optimized and found to be one cycle, dichloromethane, vortex mixing and 1.0 min, respectively. Upon obtaining the optimal conditions, the analytical performance measurements of the system were computed. The limit of detection, quantification and the correlation regression values were found to be 6.91, 23.05 µg kg^{-1} and 0.9989, respectively. Recovery tests were conducted on synthetic urine samples within the established linear working range, 33.15–505.66 µg kg^{-1}. The SA-LPME-GC-MS method was effectively utilized to the synthetic urine samples and the percentage recovery values were within the range of 90.0–105.9%.

Keywords: flibanserin; spray-assisted liquid phase microextraction; gas chromatography-mass spectrometry; synthetic urine samples

Analytical Chemistry (AC-O-008)

Combination of digital image-based colorimetric system and UV-Vis spectrophotometry for the determination of iron (III) by curcumin nanoparticle based colorimetric sensor

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Iron as one of the transition metal ions is required for numerous processes in human and animal bodies, such as oxygen transport, cell formation, electron transfer, metabolism of storage, and cellular respiration [*Sustainable Chem. Pharm.* **2022**, *29*, 100782; *Mater. Today Commun.* **2021**, *28*, 102563]. In the presented study, a simple and rapid measurement system was developed for determining iron ions using curcumin nanoparticles, analyzed by UV-Vis spectrophotometry and digital image-based colorimetry. In the laboratory conditions, curcumin nanoparticles (CurN) were synthesized rapidly and simply. CurN has a distinctive color change in the presence of iron. The curcumin nanoparticle, initially light yellow, transitions to dark yellow with an increase in iron ion concentration. A decrease in the absorption signal of curcumin nanoparticles was observed with an increase in iron (III) concentration, predicated on the color alteration. The complexation between curcumin nanoparticles capable of chelation and iron ions is a potential explanation for this behavior. To achieve an ideal improvement in detection power, univariate optimization studies were conducted on method parameters including nanoparticle volume, mixing type/period, and incubation period. As an outcome of the investigations, the limit of detection and quantification values were found to be 0.23 and 0.76 mg/L, respectively. The Color Detector application was employed to convert the digital image data to RGB (red, green, and blue) color scales. To assess the applicability and durability of the suggested procedure, tea samples were utilized in recovery tests.

Keywords: iron ions; curcumin nanoparticle; UV-vis spectrophotometry; digital image-based colorimetric system; tea samples

Analytical Chemistry (AC-O-009)

MnO_2 cube-like nanoparticles based dispersive solid phase extraction method for the preconcentration of cobalt ions from basil tea samples prior to flame atomic absorption spectrometry

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The exposure of cobalt for humans can be via various ways such as food/liquid intake, air breathing and skin contact, and high exposure of cobalt leads to several health problems [*Encyclopedia of Food and Health*, **2016**, 172–178]. For this reason, the development of an analytical method for the determination of cobalt in beverages is a crucial topic to prevent negative health effects for people. In this study, MnO_2 cube-like nanoparticles based dispersive solid phase extraction (DSPE) method was proposed to preconcentrate cobalt from food samples before flame atomic absorption spectrometry (FAAS) measurement. All substantial parameters including sample volume, pH/volume of buffer, MnO_2 amount, mixing type/period and HNO_3 concentration/volume were elaborately optimized to augment the detection power of FAAS system. System analytical performance studies were performed to evaluate the limit of detection/quantitation (LOD=5.47 µg/kg and LOQ=18.24 µg/kg), linear working range (between 10.11 µg/kg and 262.07 µg/kg) and coefficient of determination (R^2=0.9918) for the proposed method. After, applicability and accuracy for the developed method were carried out by acquiring recovery experiments with the spiked basil tea samples. Acceptable percent recovery results were calculated in the range of 96.7%–118.84% via the implementation of matrix–matching calibration strategy.

Keywords: cobalt; dispersive solid phase extraction; basil tea; MnO_2 nanoparticles

Analytical Chemistry (AC-O-010)

Accurate measurement of selected steroid hormones using a combination of the dispersive solid phase extraction method and the quadrupole isotope dilution strategy

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The key substances for the regulation of a wide range of vital body functions are steroid hormones [*J. Steroid Biochem. Mol. Biol.* **2019**, *192*, 105389; *J. Clin. Med.* **2022**, *11*, 956]. In order to understand the mechanism of steroid hormone related disorders, it is important to determine low levels of steroid hormones [*Talanta* **2021**, *224*, 121923; *Anal. Lett.* **2023**, 1–144]. In this study, Fe_3O_4/reduced graphene oxide (Fe_3O_4/rGO) nanocomposite based dispersive solid phase extraction (DSPE) was coupled with quadrupole isotope dilution mass spectrometry (ID^4MS) for the precise/accurate determination of 17-hydroxyprogesterone, testosterone, estrone and aldosterone in serum sample. Fe_3O_4/rGO nanocomposite based DSPE procedure was developed for the preconcentration of steroid hormones. The combination of the DSPE and LC-ID^4-MS/MS techniques for the extraction and identification of specific steroid hormones has not been studied in the literature. In combination with the ID^4MS strategy, significant improvements in the accuracy and precision of the proposed method have been achieved. The percent recoveries calculated were found between 100.0–103.4% with very low percent relative standard deviation values [*Anal. Methods* **2025**, *17*, 256–264].

Keywords: hormones; isotope dilution mass spectrometry; dispersive solid phase extraction; serum

Analytical Chemistry (AC-O-013)

Synthesis of $SiO_2@TiO_2@rGO@Fe_3O_4$ nanocomposites using silica nanoparticles prepared from rice husk and development of a magnetic dispersive solid phase extraction method for the determination of cadmium ions

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Cadmium (Cd) is one of the most toxic heavy metals, and exposure to it can cause significant health problems [*At. Spectrosc.* **2025**, *324*, 191–200]. This study aimed to develop an effective analytical strategy that allows the determination of Cd ions at trace levels to monitor Cd intake. For this purpose, silica nanoparticles (Si-NP) were synthesized from rice husks in the first stage [*Water. Air. Soil Pollut.* **2021**, *232*, 1–10]. Subsequently, $SiO_2@TiO_2@rGO@Fe_3O_4$ nanocomposites (NCs) were synthesized from Si-NPs. The obtained nanocomposite was characterized by evaluating morphology and compositional structure (XRD, FT-IR, and ICP-MS). The potential of Si-NPs, $SiO_2@TiO_2@rGO$ NCs and $SiO_2@TiO_2@rGO@Fe_3O_4$ NCs for the preconcentration of cadmium ions was investigated. The highest preconcentration was achieved when $SiO_2@TiO_2@rGO@Fe_3O_4$ NCs were used. Each parameter influencing the adsorption and desorption of Cd ions $SiO_2@TiO_2@rGO@Fe_3O_4$ NCs was optimized using the univariate optimization method. The optimum adsorption parameters were determined as 20.0 mg $SiO_2@TiO_2@rGO@Fe_3O_4$ NCs, 40.0 mL standard solution, 1.0 mL buffer solution and 1.0 min ultrasonication. When the analytical performance of the system was investigated, the limit of detection and limit of quantification of the developed method were found to be 0.23 µg/kg and 0.76 µg/kg, respectively. In the recovery study carried out on lemongrass tea samples using the matrix matching strategy, the percentage of recovery was calculated in the range of 89.22–108.90%. As a result of all experimental studies, a magnetic dispersive solid phase extraction method with high accuracy and sensitivity, which can be applied to several matrices, has been developed to determine trace levels of cadmium ions.

Keywords :magnetic dispersive solid phase extraction; cadmium ions; nanocomposite; characterization; preconcentration

Analytical Chemistry (AC-O-016)

Detection of tetracycline with a CRISPR/Cas12a aptasensor using a highly efficient fluorescent polystyrene microsphere reporter system

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CRISPR-based diagnostics use the CRISPR-Cas system transcleavage activity to identify specific target sequences. When activated, this activity cleaves surrounding reporter molecules, producing a detectable signal. This technique offers high specificity, sensitivity, and rapid detection capabilities, making it an important molecular diagnostic tool for medical and infectious disease applications. Despite its potential, the current CRISPR/Cas system faces challenges due to the low stability and limited sensitivity of its single-stranded DNA reporters, restricting effective application in complex biological settings. In this work, we investigate the *trans*-cleavage activity of CRISPR/Cas12a on substrates utilizing fluorescent polystyrene microspheres to detect tetracycline. This discovery led to the development of microsphere probes that enhance the stability and sensitivity of CRISPR/Cas biosensing. By attaching the ssDNA reporter to polystyrene microspheres, we discovered that the Cas12a system exhibits robust and sensitive trans-cleavage activity. Further work revealed that the trans-cleavage activity of Cas12a on the microsphere surface is significantly dependent on the concentration of the ssDNA reporters. Building on these intriguing discoveries, we developed microsphere-based fluorescent probes for CRISPR/Cas aptasensors, which showed stability and sensitivity in tetracycline biosensing. We demonstrated a highly sensitive detection of tetracycline with a detection limit of 0.1 µM. Finally, the practical use of a microsphere-based CRISPR/Cas aptasensor in spiked food samples was proven successful. These findings highlighted the remarkable potential of microsphere-based CRISPR/Cas aptasensors for biological research and medical diagnosis.

Keywords: tetracycline; CRISPR/Cas; Cas12a; amplification free; polystyrene microspheres; aptasensor; fluorescence

Analytical Chemistry (AC-O-017)

Cadmium removal from aqueous solutions with magnetite based covalent organic frameworks: Adsorption kinetics and isotherm studies

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Addressing the needs of industry requires metal processing and applications. Even low concentrations of cadmium, originating from metal ore processing, fossil fuels, and waste incineration, are detrimental. Cadmium emissions harm terrestrial and marine environments, as well as human health [*Caspian. J .Intern. Med*. **2017**, *8*, 135–145]. In this study, covalent organic framework-based adsorption procedure has been developed to remove cadmium from aqueous solutions using Fe_3O_4@COF nanomaterial. The interaction between the synthesized material and the pollutant was optimized using a 'one-factor-at-a-time' methodology to enhance cadmium removal. The interaction rates between material and pollutants increased with the optimization of parameters including pH of the aqueous solution and the amount of nanomaterial utilized. Adsorbent amount of 50 mg and solution's pH adjusted to 9.0 were found to provide the most efficient removal efficiency where Qe (adsorption capacity at equilibrium was calculated as 8.4 (mg/g). Flame atomic absorption spectrometry has been employed to analyze the target contaminant quantitatively. Prior to deploying the method, lake water samples were utilized to construct calibration plots to assess the removal efficiency. Optimal conditions were utilized to evaluate the method's pollutant removal effectiveness and adsorbent capacity across various concentrations. Adsorption isotherm models were used to compare model predictions with experimental data. The results indicated that synthesized material efficiently adsorbs the pollutant from aqueous solutions and provides high removal efficiencies fitting both monolayer and multilayer adsorption isotherms. The reusability of the synthesized material has been evaluated, yielding satisfactory results providing acceptable removal efficiency for at least 3.0 cycles.

Keywords: heavy metal; covalent organic framework; adsorption; adsorption kinetics

Analytical Chemistry (AC-O-019)

Determination of inorganic pollutants at trace levels in Antarctic region with accurate and sensitive analytical methods

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Antarctica, the most important part of the Earth's climate and ecosystem, is today a unique continent, the culmination of a long geological history. Although the amount of anthropogenic activities causing pollutants entering Antarctica is small, pollutants are highly susceptible to accumulate there due to low temperatures that inhibit evaporation. This leads to high levels of these pollutants being present in the environment and reaching food chains through biomagnification [*Sci. Total. Environ.* **2008**, *400*, 212–226]. Considering all these factors, the determination of organic/inorganic (heavy metals including cadmium, cobalt, copper, nickel) pollutants in the Antarctic region with high sensitivity and accuracy has become a vital need to protect the future of the region and the Earth. However, these contaminants can be present in environmental samples at very low concentrations that are not easily detected by conventional analytical techniques. In recent years, both solid and liquid extraction methods have been used to achieve procedures that require less time and experimental time. For this purpose, developing sensitive and innovative analytical methods for the determination of trace analytes using both chromatographic and spectrophotometric techniques that provide accurate and precise results, and the determination of these analytes in environmental samples (soil/rock, water and seaweed) makes it possible to take protective and preventive action. As a result of these developed techniques, the detection limits of the targeted organic analytes were varied between 1.0 and 6.6 ng/g. [*ESPR* **2024**, *31*, 10920–10933]

Keywords: Antarctica; pollutants; microextraction; expedition; polar region

Analytical Chemistry (AC-O-022)

Determination of zinc, cadmium, lead and copper in the acetic acid extract of food-contact plastic utensils by using square wave anodic stripping voltammetric method

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A square wave anodic stripping voltammetric method has been developed for determination of cadmium, lead, copper and zinc in acetic acid extract of food-contact plastic utensils. An aliquot of 4%v/v acetic acid solution was kept in a plastic utensils for 30 minutes in electric oven, then 10 mL of the extracted solution was placed in a voltammetric cell. The deposition of the metals was carried out by applying a constant potential of -1.30 V vs Ag/AgCl to the hanging mercury drop electrode (HMDE) for 45 s. A square wave waveform was scanned from -1.20 to 0.07 V and a voltammogram was recorded. A standard addition procedure was used for quantification. Detection limits of 0.23, 0.27, 0.32 and 0.51 µg L^{-1} for zinc, cadmium, lead and copper, respectively, were obtained. Percentage recoveries obtained by spiking 5 µg L^{-1} of each metal to the sample solution were in the range of 96 -106%. The method was successfully applied to plastic utensils which were sold in Thailand. It was found that the contents of zinc, cadmium, lead and copper released from the samples were lower than the regulated values of the Thailand industrial standard (TIS 655-2553). The proposed method is simpler, more convenient and more sensitive than the standard method based on AAS.

Keywords: food-contact plastic utensils; voltammetry; Thailand industrial standard; electrochemistry

Analytical Chemistry (AC-O-025)

Hydrothermal synthesis of bismuth ferrite nanoparticles for the determination of copper in grape leaf samples

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Bismuth ferrite ($BiFeO_3$) is a multifunctional material with significant potential in various analytical applications due to its unique properties, such as high chemical stability and adsorption capacity [*Molecules* **2024**, *29*, 3592]. Heavy metal contamination, particularly copper in food matrices, poses significant risks to human health and requires accurate detection methods [*Environ. Sci. Pollut. Res.* **2022**, *29*, 3230–3245]. In this study, bismuth ferrite ($BiFeO_3$) nanoparticles were successfully synthesized using the hydrothermal method for the determination of copper in grape leaf samples by Flame Atomic Absorption Spectroscopy (FAAS). The nanoparticles were synthesized by mixing appropriate amounts of $Bi(NO_3)_3$ and $FeCl_3$, adjusting the pH to 10, and heating the mixture at 180°C for 10 hours in an autoclave. The synthesized nanoparticles were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), and dynamic light scattering to confirm their crystalline structure, morphology, and particle size distribution, respectively. The resulting nanoparticles had an average particle size of 185.8 nm, as determined by dynamic light scattering (DLS). Analytical performance parameters, including limit of detection (LOD), limit of quantification (LOQ), linear working range, correlation coefficient (R^2), and relative standard deviation (RSD), were determined as 1.79 µg/L, 5.98 µg/L, 5.0–100 µg/L, 0.9994 and 8.7%, respectively. Experimental results demonstrated that their high adsorption capacity, combined with their large surface area, enhances copper ion interaction, thereby improving sensitivity and selectivity in analytical applications. Recovery studies were performed using a matrix-matching strategy to eliminate possible interferences, with grape leaf samples as a real sample matrix, resulting satisfactory results within the working range. These results demonstrate the potential of $BiFeO_3$ nanoparticles as an efficient material for the determination of copper in food matrices.

Keywords: bismuth ferrite; hydrothermal synthesis; copper; grape leaf; flame atomic absorption spectrometry

Analytical Chemistry (AC-O-027)

Trace determination of cadmium in cinnamon tea samples using waste toner particles based dispersive solid phase extraction

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The detrimental effects of heavy metal pollution on human health and the environment have reached alarming levels around the world. Cadmium is a toxic metal with widespread use in different industrial applications [*Int. J. Environ. Res. Public Health* **2020**, *17*, 3782]. Since long-term exposure to even low concentrations of cadmium can result in fatal diseases, the determination of cadmium at trace levels with high accuracy has long been a research topic in analytical chemistry [*Anal. Sci.* **2022**, *38*, 843–849]. In this study, a dispersive solid phase extraction (DSPE) method was developed for sensitive and accurate determination of cadmium in trace levels in cinnamon tea samples by flame atomic absorption spectrophotometry (FAAS). Waste toner particles from printer cartridges were used as sorbent material. The parameters directly affecting the extraction efficiency such as pH, buffer solution volume, sorbent mass, sample volume, mixing type and period, and eluent concentration and volume were optimized univariate approach. Under optimal conditions (24 mL of sample, 0.50 mL of pH 8.0, 45 mg of toner nanoparticles, mixing of 7.5 min of ultrasonication + 15 s of vortex and 100 µg L^{-1} of 1.0 M of HNO_3) the limit of detection (LOD) and limit of quantitation (LOQ) were found to be 0.55 and 1.82 µg L^{-1}, respectively. The linearity was obtained between 1.5 and 40 µg L^{-1} and the coefficients of determination of the calibration plots of each system were greater or equal to or greater than 0.9988. The applicability of the proposed method in real samples was investigated through recovery studies with cinnamon tea samples. To improve measurement accuracy and minimize possible matrix effects, the matrix matching calibration was applied, and acceptable recovery results were calculated between 90.4 and 119.0%. These results showed that the developed DSPE-FAAS method was feasible for the cinnamon tea and similar matrices.

Keywords: cadmium; microextraction; waste toner; spectroscopy

Analytical Chemistry (AC-O-041)

Development of biopolymer-based artificial antibodies for analytical applications

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Molecular imprinting technology enables the creation of synthetic recognition materials through a lock-and-key mechanism, forming selective and stable molecularly imprinted polymers (MIPs). These materials serve as alternatives to natural antibodies in sensors, drug delivery, and separation processes.

Recently, imprinting technology has expanded to MIP membranes (MIMs), which integrate the selectivity of MIPs with the mechanical properties of membranes. Unlike conventional MIP synthesis, which relies on high-energy inputs and costly or hazardous reagents, a novel approach using alginate and cellulose acetate as both the polymer and membrane matrix was developed in our laboratory. However, research has been limited to only a few biopolymers.

In this work, we propose a generic strategy for bio-based MIM fabrication using various biopolymers, such as cellulose derivatives, sodium alginate, chitosan, and gelatin. Additionally, MIM-based sensor arrays integrated with smartphones were successfully developed for the colorimetric detection of caffeic acid in fruits, with RGB spectral data analyzed via machine learning.

This study paves the way for sustainable, cost-effective, and highly selective artificial antibodies, promoting an eco-friendly future for imprinting technologies.

Keywords: molecularly imprinted membrane; biopolymer; non-specific adsorption; cross-linking; sensor array

Analytical Chemistry (AC-O-042)

HPTLC-derived database for phenolic compound identification in honey: Development and application

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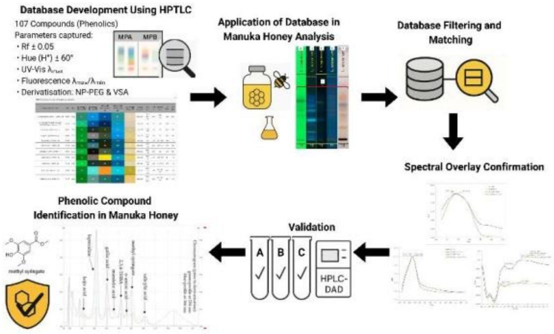
This study presents the development and validation of a high-performance thin-layer chromatography (HPTLC)-derived database for identifying phenolic compounds in honey. The database includes profiles of 107 standard compounds, capturing Rf values, fluorescence and UV-Vis spectral data, and derivatization-induced color changes. A filtering algorithm was implemented using Rf ±0.05, hue values ±60°, and UV-Vis/fluorescence λ_{max} ±15 nm (±60 nm post-derivatization) to match unknown compounds. Validation was conducted using artificial honey spiked with known and unknown compounds, and cross-validation was performed with High-Performance Liquid Chromatography coupled with Diode Array Detection (HPLC-DAD), a sensitive and widely accepted reference technique for compound quantification and spectral confirmation. Application of the method to Manuka honey led to the identification of leptosperine, mandelic acid, kojic acid, lepteridine, epigallocatechin gallate, gallic acid, o-anisic acid, and methyl syringate. HPTLC demonstrated advantages over HPLC-DAD, including comparable accuracy and compound identification, along with added benefits of visual profiling, spectral overlays, and simultaneous multi-sample analysis. The validated database provides a cost-effective and reliable tool for honey authentication and quality assessment, with compound identification confirmed through HPTLC spectral matching—covering Rf values and UV-Vis spectra under three conditions—and cross-validation with HPLC-DAD. Validation compounds showed accurate matches with no false identifications, reinforcing the method's reliability. The approach is adaptable to other natural products, offering a versatile tool for food authentication and natural products research.

Keywords: HPTLC; honey authentication; phenolic compounds; chromatographic database; Manuka honey; food quality control



Chemistry for Energy and Environment (CE-O-010)

Novel Bi-based nanocomposites for efficient photocatalytic CO_2 reduction and pollutant degradation

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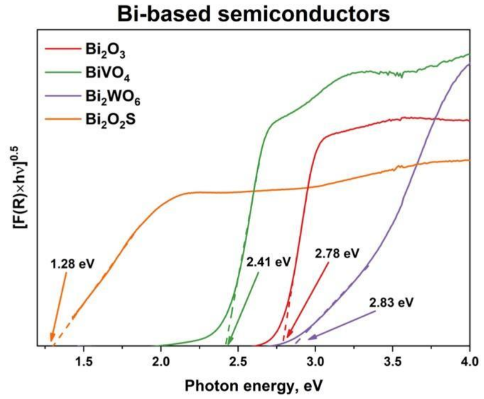
Photocatalysis has great potential in efficient utilization of light energy because photocatalytic processes ensure environmental protection, energy conversion, and sustainable development. An efficient approach in photocatalyst design is combining several semiconductors to enhance separation of photogenerated charges due to their improved interphase transfer by heterojunction. Heterostructured nanocomposites can provide boosted photocatalytic activity due to the optimum positions of energy bands to generate charge carriers under radiation with the potentials high enough for target reactions. This talk presents the results of international joint project between RSF (24-43-00182) and NSFC (22361132537) on the rational design of composite materials based on bismuth compounds ($Bi_2O_2X_n$, Bi_2WO_6, $BiVO_4$, Bi_2O_3) and other semiconductors for efficient photocatalytic CO_2 reduction and pollutant degradation. Bismuth oxycompounds ($Bi_2O_2X_n$) exhibit significant potential for solar-driven photocatalytic CO_2 conversion due to their unique electronic properties, and we have proposed novel metal-doped heterostructures based on $Bi_2O_2X_n$ and $NiCo_2O_4$ to enhance photocatalytic CO_2 reduction performance. Otherwise, Fe-decorated heterostructures composed of Bi_2WO_6 and N-doped titania are shown to decompose rapidly volatile organic pollutants both under UV and visible light due to formation of strong oxidants (H_2O_2, OH-radicals). In all cases, correlation between physicochemical characteristics of the composites and their activity in photocatalytic reactions is comprehensively discussed.

Keywords: photocatalysis; energy conversion; CO_2 reduction; environmental remediation; synergistic effect


Bi-based semiconductors

Chemistry for Energy and Environment (CE-O-012)

Sustainable production of functional activated carbons derived from biomass: assessment for energy storage and greenhouse gas (GHG) emission

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Effective management of biomass is crucial for sustainability. Currently, we have introduced a method to convert biomass materials, such as water hyacinth and silkworm pupae waste, into high-performance activated carbons through two-step chemical doping, acetic acid-assisted hydrothermal treatment followed by zinc chloride activation. Even though the high performance of such carbons in energy storage applications has been clarified, [*J. Energy Storage*. **2023**, *72*, 108578.; *Mater. Res. Bull.* **2025**, *186*, 113347.] a sustainable process to convert wastes to materials is being developed. This study presents the developed green and facile one-step chemical doping process that uses only acid buffer solutions, acting as acid-assisted hydrothermal carbonization and base-doped thermal activation. The improved method could create an ultra-microporous structure and well-distributed nitrogen atoms on carbon surfaces, resulting in 4.0 mmol g^{-1} carbon dioxide adsorption capacity. Notably, the use of GHG calculator for solid waste (version II-2013), developed based on the IPCC 2006 guidelines, indicated that our optimized production process significantly reduces CO_2 emissions relative to landfill disposal systems. Moreover, the quantity of wastewater after the production lowered by almost 50%, compared to previous studies. This underscores the potential of our strategy as a sustainable solution for upcycling waste biomass into valuable materials for applications, contributing to a circular economy and addressing environmental challenges.

Keywords: electrochemical energy storage; biomass; hydrothermal carbonization; waste upcycling; activated carbons

Gallium-based metal-organic framework for the adsorption treatment of Per- and poly-fluoroalkyl substances

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Growing concerns about environmental contamination from Per- and poly-fluoroalkyl substances (PFAS) pollution and the depletion of drinking water resources have prompted various strategic approaches for sustainable energy and environmental protection. Perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS) are considered major PFAS compounds, and the removal of PFAS from water bodies to improve the drinking water quality is one of the most promising ways to mitigate the problem. The removal of PFAS from numerous water bodies aims to produce value-added water in aquatic systems, not only addressing water pollution but also potentially eliminating the negative impacts on human health and providing a great opportunity for green and sustainable development in energy and the environment. Initially, GaOOH was synthesized, characterized, and evaluated for its adsorption capacity, demonstrating poor performance for PFOA and PFOS. This research focuses on the development of Ga-MOF-based adsorbent systems, which are notable for their simplicity, environmental friendliness, cost-effectiveness, and high efficiency. The fabrication process employs a hydrothermal method and incorporates various organic linkers under different conditions, including solvent choice, temperature, and duration, to effectively remove PFAS. The formation of the Ga-MOFs has been characterized using several techniques, such as powder X-ray diffraction (PXRD), field emission scanning electron microscopy (FE-SEM), and Fourier-transform infrared spectroscopy (FT-IR). Additionally, the adsorption performance of these materials has been evaluated. The details of this study will be presented.

Keywords: PFAS; gallium-based MOF; adsorption; GaOOH; environment

Development of Ni-based electrocatalysts by Fe doping and carbon nanotubes coating for urea oxidation reaction

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Urea oxidation reaction (UOR) is a promising technology to produce hydrogen from urea containing wastewater. The bottleneck of UOR is sluggish kinetics because of the six-electron transfer step. To boost the UOR performance, nickel (Ni) is widely used as cost-effective, but Ni suffers from low stability and inadequate active sites. Some studies have shown iron (Fe) can promote the activity of Ni-based catalysts. Furthermore, the incorporation of conductive carbons such as carbon nanotubes (CNTs) has been shown to lower the electrode resistance and UOR overpotential. In this work, the role of CNTs and Fe on the UOR performance and durability of Ni-based catalysts was investigated in Three-Point probe cell. The CNTs were coated onto Ni foam by facile deposition followed by electrodeposition of Fe, which produced coral-like crystals attached to CNTs. Electrochemical tests (including Linear sweep voltammetry (LSV), Electrochemical Impedance Spectroscopy (EIS), Cyclic voltammetry (CV), and long-term studies) in 1 M KOH + 0.33 M urea did not show synergistic effects between Ni and Fe. However, the specific capacitance (C_{dl}) of CNTs has highest value of 3.33 mF·cm^{-2} showed a significantly increased electrochemical active surface area (ECSA). and synergistic effects between CNTs and transition metals were observed for UOR.

Keywords: carbon nanotubes; transition metals; electrodeposition; urea oxidation; oxygen evolution

Oxidative valorization of spruce bark to yield vanillin

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To create an economically viable and environmentally sustainable biorefinery, it is crucial to fully utilize all components of biomass, including the often-overlooked spruce bark. Currently, spruce bark, which accounts for about 10% of timber and pulpwood, is predominantly used as fuel, while the tops and branches, which make up to 50% of the spruce bark, remain underexploited.

This research focuses on enhancing the value of spruce bark by extracting valuable aromatic compounds from the lignin fraction using a "lignin-first" oxidative catalytic fractionation under alkaline solvent with O_2 as an oxidant in the presence of Cu(II)O as a catalyst. In this method, the lignin is selectively oxidized, leading to the formation of monophenolic compounds. The yield from this approach was 21%, which is significantly higher than the yield obtained through traditional nitrobenzene oxidation, which showed no yield. Additionally, carbohydrate pulp was successfully isolated from the residual biomass and further processed for textile fiber production, achieving a 72% conversion of spruce bark to carbohydrate pulp, which is suitable for nanocellulose production.

These findings demonstrate the potential of repurposing spruce bark, typically seen as a low-value fuel, into a high-value feedstock.

Keywords: spruce bark; oxidative catalytic fractionation; pulp; lignin first

Chemistry for Energy and Environment (CE-O-017)

Selective recovery of Mo, V, and Ni from waste inorganic resources, using ionic liquids and deep eutectic solvents

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This study presents a green and efficient method for metal recovery using ionic liquids (ILs) and deep eutectic solvents (DESs) as sustainable alternatives to traditional high-temperature or acid-based processes. A spent hydrodesulfurization (HDS) catalyst was first treated with a phosphonium-based IL to selectively extract molybdenum (Mo) and vanadium (V), while nickel (Ni) was later recovered from the residue using a DES. The IL was synthesized by reacting tetrahexylphosphonium chloride (Cy^+Cl^-) with a phosphoric acid ester (D2EHPH), producing Cy-D2EH under mild conditions (25°C, 2 h) followed by $NaHCO_3$ neutralization. Vanadium and molybdenum were subsequently precipitated as NH_4VO_3 and $BaMoO_4$, respectively, while Ni was recovered via cementation with aluminum. DESs were formed from hydrogen bond acceptors, e.g., phosphonium chlorides, and donors such as para-toluene sulfonic acid (PTSA) and ethylene glycol, enabling selective extraction through hydrogen bonding interactions. This dual-solvent system eliminates the need for roasting or harsh chemical treatments and demonstrates high selectivity, reusability, and low toxicity, making it highly suitable for sustainable metal recycling.

Keywords: ionic liquid; deep eutectic solvent; recycling

The effect of the carbon-to-silica template mass ratio on the performance of mesoporous carbon derived from banana peel as a supercapacitor

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This study investigates mesoporous carbon derived from banana peel waste for supercapacitor applications. The material was synthesized using banana peel powder as the carbon precursor, along with MCM-41 and silica gel 60 (SG-60) as hard templates. The synthesis involved the hydrothermal impregnation of banana peel powder with different templates at varying carbon-to-silica mass ratios, followed by carbonization under an N_2 atmosphere and washing with NH_4F solution to obtain mesoporous carbon (MC-M and MC-S). The synthesized mesoporous carbon was characterized using TGA, FTIR, XRD, XRF, Raman, TEM, and N_2-physisorption to determine its properties. The mesoporous carbon assisted by MCM-41 (MC-M) and the mesoporous carbon at a carbon-to-SG60 ratio of 3:1 (MC-S-3) exhibited the highest specific surface areas. Electrochemical performance of the synthesized mesoporous carbon, with nickel foam as the supporting electrode, was evaluated using cyclic voltammogram, galvanostatic charge-discharge, and electrochemical impedance spectroscopy in a 3.0 M KOH electrolyte. The MC-M@NF and MC-S-3@NF materials exhibited the highest specific surface areas, indicating a correlation between surface area and specific capacitance. Additionally, the electrode exhibited stable performance over 2500 voltammetric cycles, confirming that MCM-41 and SG-60 are effective hard template for synthesizing mesoporous carbon from biomass.

Keywords: mesoporous carbon; hard template; silica gel 60; MCM-41; supercapacitor

Chemistry for Energy and Environment (CE-O-025)

Optimization of ammonia fuel cells using two dimensional NiFe-MOF/NF as electrodes

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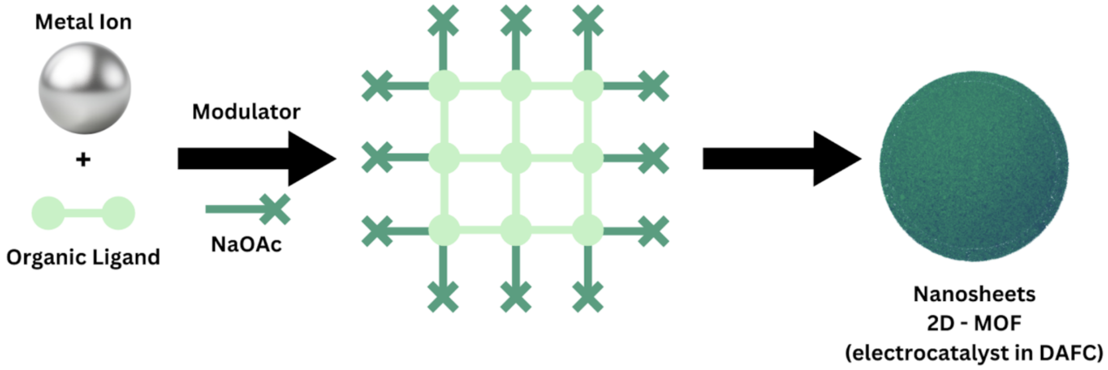
This study aims to explore the synthesis of two-dimensional bimetallic Metal-Organic Frameworks (MOFs) as electrode catalysts for ammonia-based fuel cell applications. The synthesized catalyst, a two-dimensional NiFe-MOF, is deposited onto nickel foam to enhance its catalytic properties. The synthesis process involves the addition of modulators such as sodium acetate (NaOAc), which acts as an interruptor to regulate the stacking of MOF layers during formation. Material characterization is carried out using Scanning Electron Microscopy (SEM), Fourier-Transform Infrared Spectroscopy (FT-IR), and X-Ray Diffraction (XRD) to analyze the structure, morphology, and composition of the synthesized MOF. The two-dimensional NiFe-MOF, with its high surface area and more exposed active sites, serves as an anode catalyst to improve the electrochemical performance of Direct Ammonia Fuel Cells (DAFC). Given its efficiency in facilitating ammonia oxidation, this study highlights the potential of ammonia fuel cells as a long-term solution for sustainable energy, offering a cleaner and more efficient alternative in the transition toward renewable energy technologies.

Keywords: direct ammonia fuel cell; two-dimensional bimetal MOF; nickel foam; NiFe-MOF



Chemistry for Energy and Environment (CE-O-031)

Ecological risk assessment and pollution study of the lifeline river adjacent to the megacity Chattogram, Bangladesh

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The Karnafuli River, serving as the lifeline of Chattogram, Bangladesh, is under growing threat from rapid urbanization, industrial activities, and unregulated waste discharge. This study aimed to assess the pollution status and ecological risks associated with the river's water quality to inform sustainable management strategies. Water samples were systematically collected from nine strategically selected sites—upstream, industrial, urban, and estuarine areas—across three distinct seasons (pre-monsoon, monsoon, and post-monsoon) during the hydrological years 2021–2022, totaling 27 samples. Standard procedures outlined by the American Public Health Association (APHA, 2017) were employed to measure key physico-chemical parameters including Temperature, pH, Dissolved Oxygen (DO), Total Dissolved Solids (TDS), Total Suspended Solids (TSS), Conductivity, Biological Oxygen Demand (BOD), Chemical Oxygen Demand (COD), Total Hardness, Alkalinity, Chloride, Carbon Dioxide (CO_2), and Acidity. Data were statistically analyzed using descriptive statistics and compared against national and WHO water quality standards. Results revealed significant spatial and seasonal variations: industrial and estuarine sites recorded extremely high TDS (up to 21,785 mg/L) and Conductivity (up to 42,400 µS/cm), while DO concentrations frequently dropped below 4 mg/L, signaling ecological stress. Elevated BOD (up to 4.5 mg/L) and COD (up to 99 mg/L) levels indicated organic pollution, particularly in urban and industrial zones. Several parameters exceeded safe limits, posing risks to aquatic ecosystems, human health, and agricultural activities. The findings highlight the urgent need for pollution control, effective wastewater management, and continuous environmental monitoring to protect the Karnafuli River's ecological integrity.

Keywords: physico-chemical parameters; water quality; climate change; Karnaphuli river; Bangladesh

$ZnCl_2$-activated porous biochar from fast-growing flowering plant, Wolffia as lithium-ion batteries anode materials

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Wolffia or “Khai-num” in Thailand, is a high biomass yield resource that benefits energy and future human food production. In this research, the porous biochar from this outstanding plant assisted with a $ZnCl_2$ pore activator was studied as the next alternative sustainable biomass-based anode material for lithium-ion batteries. The biochar with a low crystallinity carbon phase was easily obtained when pure Wolffia or Wolffia with $ZnCl_2$ was carbonized at 800 °C. Compared with pure biochar (WF-800), the surface of $ZnCl_2$-activated biochar (WF2-800) was seriously eroded, revealing the mesopore and macropore structures as observed under FESEM and TEM. Moreover, the specific surface area of the pure biochar was enormously enhanced from 37 m^2/g to 1,064 m^2/g after $ZnCl_2$ activation. As a result of the three-size pore structures with high specific surface area in WF2-800, the electrochemical performance as the lithium-ion batteries anode was significantly improved. WF2-800 has an excellent specific capacity of 394 mAh/g, while the pure biochar has only 264 mAh/g after 100 cycles at 100 mA/g. Compared to current commercial graphite, this work clearly showed that the enhanced capacity anode material with high stability could be simply prepared from a sustainable biomass-based carbon source assisted with a $ZnCl_2$ pore activator.

Keywords: Wolffia; sustainable biomass; $ZnCl_2$; porous biochar anode; Li-ion batteries

Oxygen harvesting waste derived carbon dots as photocatalysts for the oxidative synthesis of quinazolinones

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A protocol for the synthesis of quinazoline-4(*3H*)-ones from alcohol precursors is important for the pharmaceutical industry as current approaches need transition metal catalysts and high temperatures. Herein, waste plastic-derived carbon dots (CDs) have been used for the one-pot synthesis of quinazoline-4(*3H*)-ones as an inexpensive metal-free photocatalyst with high efficiencies, including five potent drug molecules and established the reaction mechanism. To add to the benefits, the unique oxygen harvesting properties of the CDs are shown to facilitate the use of molecular O_2 present in ambient air as an inexpensive but highly facile oxidant for oxidative synthesis. The protocol eliminates the need for external oxidants, ligands, or additives and enables identical efficiencies in air and oxygenated atmospheres, paving the way for using air in industrial processes. This is an example of photochemical synthesis of the widely used quinazolinone-based drug molecules where the utilisation of waste plastics as feedstock in catalyst synthesis makes it even greener.

Keywords: waste treatment, carbon dots, quinazolinones

Food, Agriculture, and Cosmetics (FA-O-001)

Application of photopharmacology in agrochemicals

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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, GluCls, 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

Significance of yield and phytochemical analysis of tea plant (*Camellia sinensis* (L.) O. Kuntze) in different rainfall in West Java plantation

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The tea productivity contributes to national revenue due to its high selling price in international markets. However, the increasing market demand conflicts with fluctuating production caused by extreme climate changes. This study, conducted at the Experimental Field at the Center for Tea and Cinchona Research in Gambung, Ciwidey, West Java, Indonesia, approximately 1,350 meters above sea level, from October 2023 to March 2024, aimed to address this challenge. A plot design used various rainfall as treatments and each harvest time as replications. Quantitative descriptive methods, including t-test and correlation coefficient analysis, were conducted. The observations included yield, bud number, leaf picking efficiency, soil moisture, precipitation, temperature, humidity, and total phenolic contents (TPC) and total flavonoid content (TFC) as phytochemical variables. The results showed soil moisture was higher during the rainy season, promoting vegetative growth and affecting yield. The TPC and TFC composition in the rainy season is also higher than in the dry season. Seasonal variations significantly impacted productivity and quality of tea, with dry seasons showing lower results. Rainfall and humidity positively correlated with tea productivity, while temperature negatively affected it. Seasonal influences remain critical in determining the yields and quality of tea plants.

Keywords: production; phytochemical; tea plant; rainy seasons; dry seasons

Food, Agriculture, and Cosmetics (FA-O-003)

From zap to map: How vibrational spectroscopy characterizes PEF-induced changes and rapidly predicts protein content in semi-refined flaxseed extract

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This study investigates pulsed electric field (PEF) technology as an enhanced extraction strategy for flaxseed, an emerging high-quality plant protein source and functional food ingredient. Raman spectroscopy coupled with principal component analysis (PCA) generated distinctive spectral fingerprints that revealed specific structural alterations in protein secondary and tertiary conformations across different PEF treatments. Complementary scanning electron microscopy (SEM) confirmed these findings by visualizing β-sheet aggregation patterns in both control samples and those subjected to high-intensity PEF treatment (~534 kJ/kg). For protein quantification, micro near-infrared (NIR) spectroscopy demonstrated fast and accurate prediction. The application of second derivative and standard normal variate (SNV) preprocessing significantly enhanced predictive model performance across diverse sample matrices (root mean square error of prediction ($RMSE_P$): 0.09% and ratio of performance deviation (RPD): 8.26) when validated against the Dumas method. Moderate PEF treatment (up to 347 kJ/kg) enhanced protein extraction without requiring higher pH, while higher energy inputs (~347–534 kJ/kg) in alkaline conditions increased phenolic compound extraction. These findings contribute to the development of sustainable protein processing and characterization technologies, offering potential valuable applications across the plant-based protein industry.

Keywords: chemometrics; flaxseed; microNIR spectroscopy; pulsed electric field; Raman spectroscopy

Food, Agriculture, and Cosmetics (FA-O-004)

Optimizing tea plant growth and total phenolic content recovery through biofertilization and fertilization strategies after drought

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The crucial post-drought condition of tea plants requires optimal strategies to recover and improve quantity and quality. Biofertilizers contain microorganisms that can support post-drought tea plant growth by providing nutrients and phytohormones. The experiment was conducted at the Tea and Cinchona Research Center, Gambung, Ciwidey, from January 2024 to August 2024, used a split-plot design. The main plot consisted of 2 levels of fertilization techniques, subplots consisted of 4 levels of fertilizer dosage, repeated 3 times. The main plot consisted of foliar spraying and poured onto the soil treatments, while the subplots consisted of biofertilizer dosage treatments of 0 L ha^{-1}, 15 L ha^{-1}, 22.5 L ha^{-1}, and 30 L ha^{-1}. Total Phenolic content (TPC) determined by Folin-Ciocalteu method. The results showed an interaction, application of poured onto the soil with a dose of biofertilizer of 15 L ha^{-1} produced the highest fresh shoot weight at the 3rd harvest. Similarly, soil drenching with 15 L ha^{-1} biofertilizer dose produced the highest TPC in the 2nd, 3rd, and 6th harvests. Microorganisms in biofertilizers adapt to tea soil and increase antioxidants. Microorganisms release phenylpropanoids, which trigger redox reactions, affect enzymatic activity, and increase the availability of phytonutrients and hormones.

Keywords :biofertilizer; fertilization techniques; post-drought; polyphenol content; recovery

Inorganic Chemistry (IC-O-002)

Ru(II)/diphosphine-naphthoquinone complexes as anticancer agents

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The incorporation of ligands that increase lipophilicity of the complexes (potential drugs) is a good strategy for the development of metallodrugs. Thus, natural products, presenting biological activities, emerge as a promising class of interesting ligands. Recently, we have used this strategy and natural products have been chosen to obtain active ruthenium complexes against several type of cancer cells. Here we synthesized and characterized complexes containing a naphthoquinone derivative as ligand: [Ru(NQ1)(bipy)(dppen)]PF_6 (**1**), [Ru(NQ2)(bipy)(dppen)]PF_6 (**2**), [Ru(NQ1)(bipy)(DPEPhos)]PF_6 (**3**), and [Ru(NQ2)(bipy)(DPEPhos)]PF_6 (**4**) (bipy = 2,2'-bipyridine, dppen = 1,2-bis(diphenylphosphino)ethylene, DPEphos = bis[(2-diphenylphosphino)phenyl]ether, and NQ1 and NQ2 = deprotonated lawsone and lapachol, respectively. *In vitro* assays showed that complexes 1–4 are cytotoxic against MDA-MB-231, SK-BR-3, and MCF-7 breast cancer cells. The non-tumoral breast cells MCF-10A was also tested and these complexes provided lower IC50 than cisplatin, used as control. The complexes showed good selectivity indexes for the triple negative breast cancer cell line MDA-MB-231, inhibited colony formation, induced the apoptosis, and arrested them in the G2/M phase of the cell cycle. 1–4 interacted with ct-DNA via minor groves and presented moderate binding affinity for HSA. FAPESP (2023/02475-8) and CNPq (401770/2023-0).

Keywords: ruthenium(II); diphosphine; naphthoquinone; anticancer agents

Inorganic Chemistry (IC-O-007)

Voltammetric behavior of Keggin-type vanadium-containing poltoxometalates: Redox sites and redox kinetics

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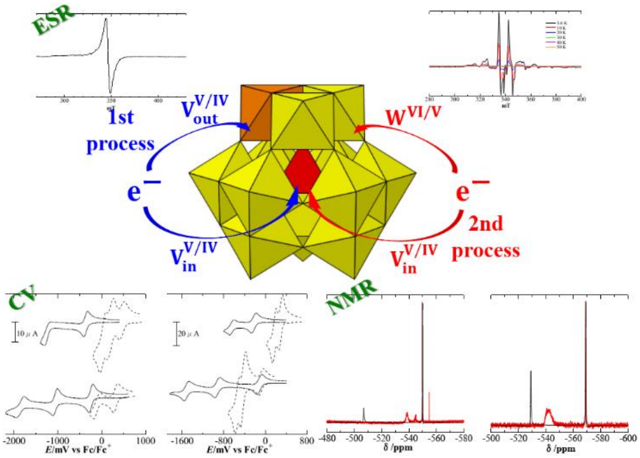
Polyoxometalates(POMs) are inorganic clusters, which are composed of tungsten and molybdenum as framework parts and silicon and phosphorus as central parts and oxygen. They exhibit fascinating chemical properties such as strong acidity, less corrosiveness, multi-electrons accommodation and bioactivity leading to the application to various fields: catalysts, battery materials and sensors. However, many fundamental properties of POMs are still unclear, especially electrochemical redox mechanism. Generally, one-electron transfers occur under neutral condition where no proton coupled with Keggin-type POMs, $[XM_{12}O_{40}]^{n-}$ (X=S, P, Si; M=Mo, W), at each of redox potentials, while two-electron transfer under highly acidic conditions. Although qualitative analysis on the redox mechanism of POMs has been conducted in most cases, our group has quantitatively elucidated on redox mechanism of Keggin-type POMs by using simulation of cyclic voltammograms with a help of ESR and NMR to obtain electrochemical and chemical parameters such as acid association constants. Vanadium is substituted with some of tungsten and molybdenum parts to form vanadium-substituted POMs, e.g. $[XVM_{11}O_{40}]^{m-}$, and it is also incorporated into the central part of POMs, $[V_{in}M_{12}O_{40}]^{3-}$ and $[V_{in}V_{out}M_{11}O_{40}]^{4-}$. In this conference, I will give a presentation on the reduction sites of $[V_{in}M_{12}O_{40}]^{3-}$ and $[V_{in}V_{out}M_{11}O_{40}]^{4-}$ based on direct evidence and the electron transfer kinetics of $[V_{in}W_{12}O_{40}]^{3-}$, $[V_{in}V_{out}W_{11}O_{40}]^{4-}$ and $[SV_{out}W_{11}O_{40}]^{3-}$ by using Fourier transformed large amplitude alternative current voltammetry (FT-ACV).

Keywords: polyoxometalate; Keggin-type; simulation; cyclic voltammetry; Fourier transformed large amplitude alternative current voltammetry



Inorganic Chemistry (IC-O-008)

Discrete coordination nanochains based on photoluminescent dyes reveal intrachain exciton migration dynamics

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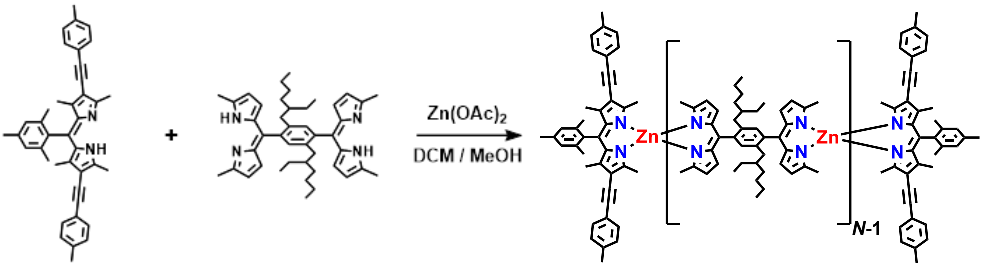
Elucidating exciton migration in polymer chains has been one of the major research goals in photophysics for over half a century. While great efforts have been made to understand picosecond phenomena by ultrafast spectroscopy, ambiguous molecular conformations and/or random polymer sequences have hindered the construction of an ideal exciton migration model. Here we present the creation of unique end-capped coordination nanochains and quantitative description of intrachain exciton migration therein. The nanochain features unique molecular architectures in discrete polynuclear complexes, with a linear and rigid structure, the defined number of metal nuclei, and charge neutrality. These features allow well-defined arrangement of emissive dye moieties, making the nanochain a sound platform for studying exciton dynamics. Readily accessible absorption spectroscopy, and photoluminescence lifetime and quantum yield measurements allow the construction of continuous-time Markov chains model, thereby estimating non-trivial exciton migration across the metal center. [*Nat Commun.* **2025**, *16*, 1367]

Keywords: dipyrrin; nanochain; zinc; exciton; continuous-time Markov chains model



Inorganic Chemistry (IC-O-010)

Insight into the delocalization of excited states in isomorphous palladium(II) and platinum(II) one-dimensional chains

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Precise control of metal-metal interactions in transition metal complexes is essential for developing advanced materials with tunable optical properties. While self-assembled Pt(II) complexes have been extensively studied for their unique optical properties arising from excited states caused by Pt···Pt interactions, a key challenge remains in the limited understanding of excited-state behavior in self-assembled Pd(II) systems, despite having the same d^8 electronic configuration.

In this work, we have explored the luminescence behavior of isomorphous Pt(II) and Pd(II) complexes, $K[M(CN)_2(dFppy)]\cdot H_2O$ (M = Pt, Pd; dFppy = 2-(4,6-difluorophenyl)pyridinate), which exhibit one-dimensional metal-metal interactions. Spectroscopic analysis revealed a striking contrast: the Pt(II) complex underwent a drastic thermochromic shift in luminescence (>100 nm), while the Pd(II) complex displayed an enhanced quantum yield upon cooling at nearly the same emission wavelength. Single-crystal X-ray diffraction confirmed subtle structural variations that govern these distinct thermos-responsive behaviors. Detailed variable-temperature studies revealed that these differences in emission properties stem from disparities in the delocalization of electron density in ^{3}MMLCT excited states through metal-metal interactions: the thermochromic shift of the Pt(II) complex results from thermal equilibrium between extensively delocalized excited states, while the emission of the Pd(II) complex originates from localized dimeric units [*Chem. Sci.* **2024**, *15*, 14497–14505].

Keywords: chromism; luminescence; metal-metal interactions; Pd(II) complexes; Pt(II) complexes

Inorganic Chemistry (IC-O-014)

Synthesis of polyesters using +2 and +3 metal complexes

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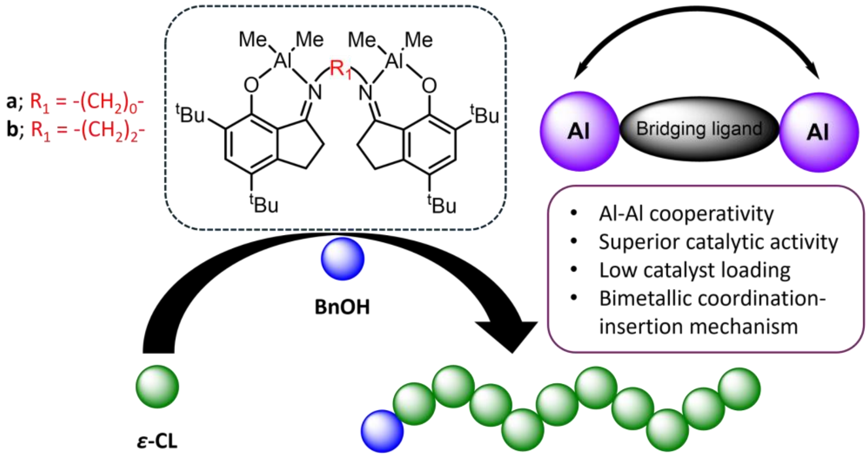
Polyesters such as polylactide and poly(ε-caprolactone) are among the most extensively studied polyesters due to their biodegradable and renewable properties. To synthesize such polymers in a controlled manner, single-site ligated metal complexes have been employed. The supporting ligands have played crucial roles to control the catalysts' activities and selectivities. In this work, +2 and +3 metal complexes (Zn, Sn, Al) supported by constrained Schiff base ligands based on substituted 7-hydroxy-1-indanone were reported. The Zn complex was found to be highly active for the ring-opening polymerization (ROP) of 500 equiv of L-lactide in 3 min at room temperature. On the other hand, Al complex is generally much less reactive. With some ligand tuning, a bimetallic Al complex can be synthesized and shown to cooperate between the two metals in the ROP of ε-caprolactone giving higher activity compared to the monometallic analogue. The work also extended to the ring-opening copolymerization (ROCOP) of cyclic anhydrides (A) and epoxides (B). The Al complexes are well-behaved producing strictly alternate $(AB)_n$ polyesters. On the other hand, the Sn complex produced a novel class of polyesters containing $(ABB)_n$ polymer sequences having superior thermal properties compared to the conventional $(AB)_n$ polymer.

Keywords: polyester; polylactide; single-site catalyst; ring-opening polymerization



Inorganic Chemistry (IC-O-019)

Tunable metal-free imidazole-benzimidazole-based electrocatalysts for oxygen reduction reaction (ORR) in water

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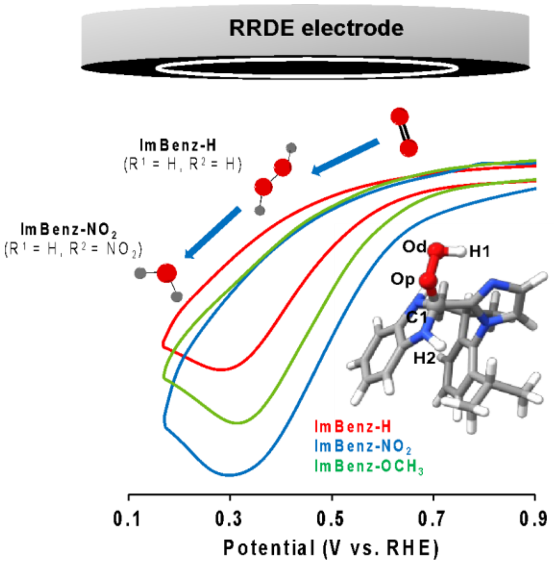
A series of metal-free imidazole-benzimidazole-based electrocatalysts with different substituents (**ImBenz-H**, **ImBenz-NO_2**, and **ImBenz-OCH_3**) were successfully synthesized through Cu-catalyzed oxidative C–N cyclization for tunable catalytic activity of electrochemical O_2 reduction (ORR) in CH_3CN and aqueous media. All ImBenz electrocatalysts demonstrated efficient ORR catalysis with onset potentials (E_{onset}) of approximately 0.63 V and 0.65 V vs RHE in pH 7 phosphate buffer (PB) and pH 13 KOH solutions, respectively. **ImBenz-NO_2**, with an electron-withdrawing group, exhibited remarkable selectivity for H_2O formation via the 4-electron ORR pathway with 3.7e$^-$ under neutral conditions. In contrast, the highest selectivity for H_2O_2 production with number of electrons transferred close to 2 was observed with **ImBenz-H** under alkaline conditions. The ORR kinetics study using FOWA indicated that **ImBenz-H** yields the highest turnover frequencies (TOFs) around 10^3 s^{-1} in both pH media. In addition, the DFT calculation disclosed the redox-active properties of imidazole-benzimidazole catalysts influencing the binding of O_2 molecules to produce H_2O_2 as a first product.

Keywords: benzimidazole; oxygen reduction reaction; metal-free electrocatalyst; redox-active; electrocatalysis



Inorganic Chemistry (IC-O-020)

A robust C_3-symmetric aluminate hydride for CO_2 hydroboration catalysis: Mechanistic insights and counter-cation influence on catalytic performance

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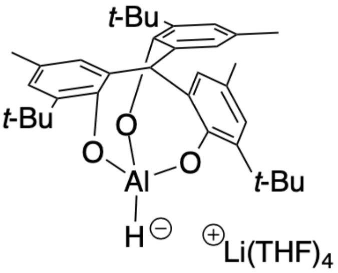
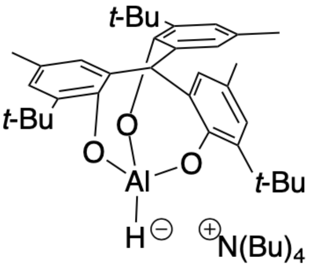
This work presents a detailed study of the synthesis, structures, and catalytic applications of robust C_3-symmetric tridentate *tris*-phenolate aluminum hydride anions, prepared as Li^+ and $[N(^n Bu)_4]^+$ salts. These compounds were characterized and evaluated for their reactivity with CO_2 and their performance in CO_2 hydroboration catalysis. The influence of counter-cation nature on catalytic activity and selectivity was assessed, supported by DFT calculations to propose a detailed reaction mechanism.

Keywords: aluminum complexes; *tris*-phenolate ligand; CO_2 hydroboration catalysis; DFT calculations





Industrial and Engineering Chemistry (IE-O-004)

Development of CO_2 capture technology using phosphonium amino acid ionic liquids (PAA-ILs) as a green absorbent for enhanced absorption efficiency

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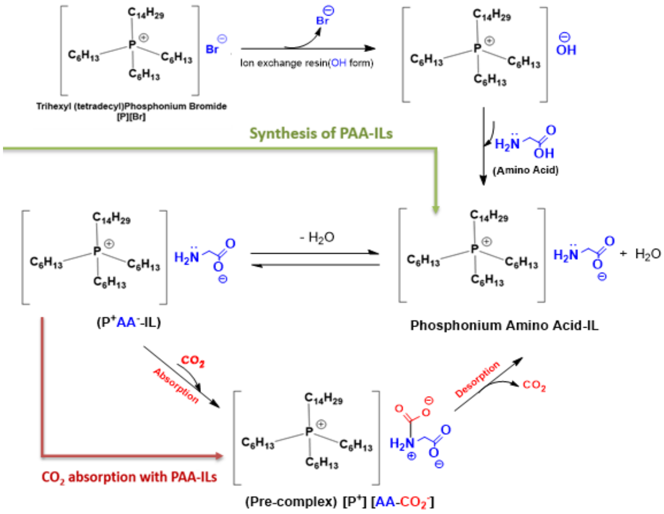
Effective CO_2 capture and emission abatement are crucial for mitigating climate change, driving the need for highly efficient and stable absorbents. This study focuses on the synthesis, characterization, and CO_2 absorption performance of trihexyl(tetradecyl)phosphonium bromide, [THTDP][Br] ionic liquid functionalized with amino acids (glycine, arginine, lysine and histidine). The phosphonium cation $[(C_6H_{13})_3(C_{14}H_{29})]P^+$ pairs with amino acid-based aminate anions $[AA]^-$ to form $[THTDP]^+[AA]^-$ ionic liquids. Synthesized and CO_2-absorbed ionic liquids were characterized using FTIR, ^1H, ^{13}C NMR spectroscopy, and viscosity analysis. CO_2 absorption studies were conducted at 3-5 bar pressures and 15–40 °C temperatures. Results indicate that functionalized ionic liquids with multiple amine sites ($-NH_2$) exhibit high CO_2 absorption capacities, ranging from 0.2 to 0.6 moles CO_2/mole ILs. FTIR spectra confirm N–H (3300–3500 cm^{-1}) and C=O (1550–1650 cm^{-1}) stretching intensities increase due to amino ($-NH_2$) and carboxyl ($-COO^-$) groups. Phosphonium stretching vibrations (2922–2858 cm^{-1}) and C-H stretching ($-CH_3$) at 1455–1462 cm^{-1} were also identified. The ^1H NMR spectrum shows a peak at δ = 3.20–3.40 ppm for the ($N-CH_2-COO^-$) group, while ^{13}C NMR confirms the carboxyl ($-COO^-$) group with a peak at δ = 180–182 ppm. These results show that the CO_2 absorption capacity of the synthesized $[THTDP]^+[AA]^-$ ILs outperforms literature values, highlighting their potential as efficient, green absorbents for CO_2 capture.

Keywords: carbon capture; phosphonium ionic liquids; amino acids; functionalization; green absorbent



Materials Science and Nanotechnology (MN-O-001)

Rare-earth metal promoters (La, Ce, Nd, Sm) on nickel-supported Al_2O_3 catalysts for ammonia decomposition

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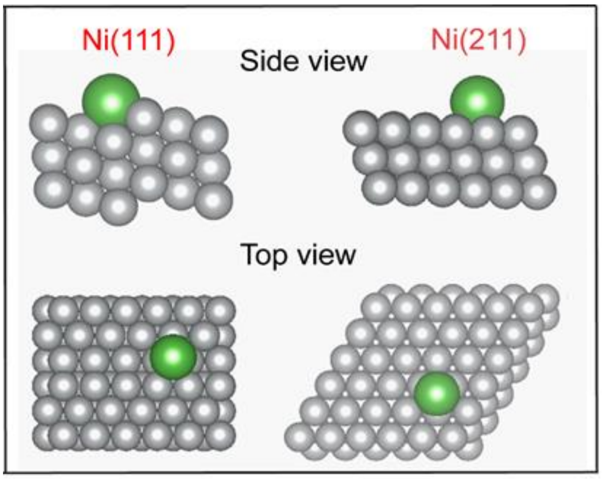
Ammonia is the 2nd most widely produced chemical, storing 17.6 wt% of hydrogen, but the economic generation of hydrogen from it needs a more affordable solution. Hence, replacing precious metals, such as ruthenium (Ru), with inexpensive nickel (Ni) is desirable. In this study, a series of rare-earth metals (La, Ce, Nd and Sm) promoted nickel nanoparticles supported on alumina (Al_2O_3) have been investigated for ammonia decomposition. Here, 3, 5 and 10% promoters loaded on Ni on Al_2O_3 have been prepared and characterized by XRD, SEM, TEM, BET, H2-TPR and XPS. HRTEM and elemental mapping reveal a homogeneous distribution of La-promoters on the surface of Ni nanoparticles with an average size within a narrow range of 31 nm. Catalyst 5%La-Ni/Al_2O_3 demonstrates 90% ammonia decomposition activity at 510°C, outperforming the 5%Ce-Ni/Al_2O_3 under the optimized gas hourly speed velocity (GHSV) of 20,400 mL/gcat/h. respectively. The 5%La-%Ni/Al_2O_3 and 5%Ce-Ni/ Al_2O_3 catalysts retained their stability for an extended period of time (65 h). The frequency of the dehydrogenation reaction of ammonia on the various Ni(211) and close-packed (111) on the alumina surface has been correlated with the density functional theory (DFT) studies, and the experimental results are corroborated accordingly.

Keywords: ammonia; ammonia decomposition; hydrogen; hydrogen storage; La promoter



Materials Science and Nanotechnology (MN-O-004)

A dual-mode biosensor with CeO_2 nanozyme mediation for RPA/CRISPR-Cas12a detection of *Salmonella* bacteria

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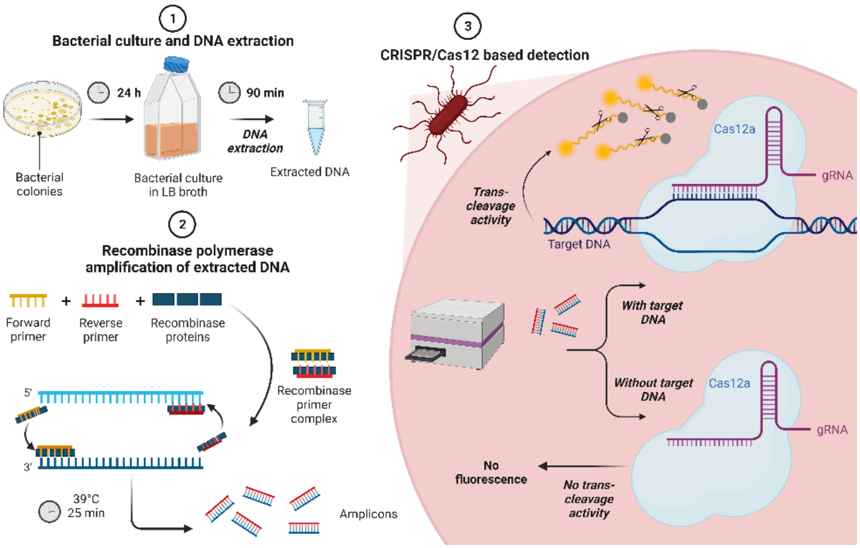
This study reports a novel biosensing system that leverages recombinase polymerase amplification (RPA) in conjunction with clustered regularly interspaced short palindromic repeats (CRISPR)/Cas12a technology, integrated with a nanozyme (NZ) based on cerium dioxide (CeO_2). With the integration of CeO_2 NZ, a dual-mode detection platform could be developed for *Salmonella* detection using fluorometric and colorimetric assays. The CRISPR/Cas12a system, when activated in the presence of target DNA, could cleave the FAM-labelled probe to lead to a fluorometric response. Also, when the CeO_2 NZ was introduced in the presence of H_2O_2, a colorimetric response was generated, directly proportional to the concentration of target DNA present. We hypothesize that adding highly reactive H_2O_2 within the post-CRISPR/Cas12a reaction system allows for an increased release of hydroxyl free radicals within the mixture. Thus, the double recognition through NZ and the CRISPR/Cas12a system provided enhanced selectivity and sensitivity. The proposed biosensor could successfully detect *Salmonella* at concentrations as low as 0.88 pg/µL and 1.28 pg/µL for fluorometric and colorimetric responses, respectively. Furthermore, the developed biosensor could be applied in real sample analysis of raw food samples to give a good recovery in the spiked food samples with varying concentrations of cultured bacterial DNA.

Keywords: nanozyme; dual-more sensor; CRISPR/Cas; *Salmonella*



Materials Science and Nanotechnology (MN-O-010)

MOF-NP interface control for catalytic selectivity regulation

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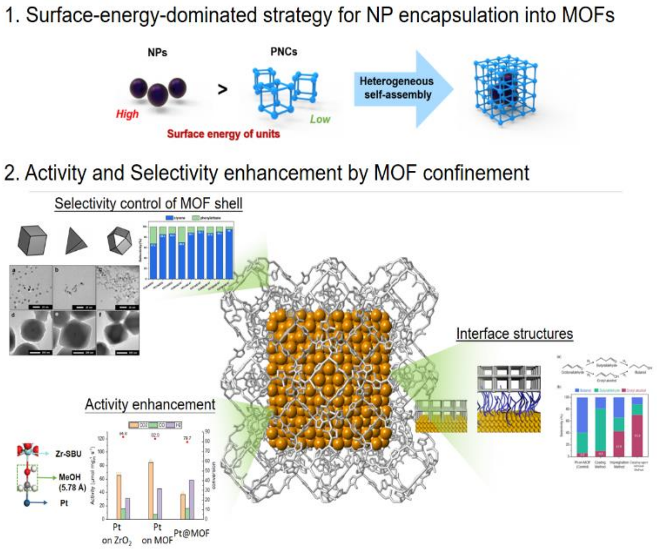
Encapsulating metal nanoparticles (NPs) in metal−organic frameworks (MOFs) to control catalytic selectivity has recently attracted great attention; however, an understanding and control over the NP-MOF interface is lacking. In this work, we developed a strategy to mediate MOF growth on the surface of NPs to control interfacial structure, by taking advantage of the various capping agents. A direct and indirect contact interface of NP-MOF can be synthesized in single-crystalline MOF shell. In addition, the surface-energy-dominated mechanism was invented to achieve the generality of this strategy in various MOFs, reaction conditions and the use of capping agents. Furthermore, we used spectroscopy to investigate the interfacial structure and then demonstrate its impact on selectivity. Chemical interactions at the interface were probed through IR and Raman spectroscopy. The different interfacial structures display a very different selectivity to several catalysis reactions. This work opens a new route to create controllable interfaces between materials and provides a feasible method for efficient NP encapsulation and sheds light on their design for effective NP-MOF catalysts.

Keywords: metal-organic frameworks; interfacial structure; structure-function relationship; catalytic selectivity; synergistic effects



Enhancement of electrocatalytic properties of Au/poly(3,4-ethylenedioxythiophene) hybrid materials by simultaneous Au electrodeposition with electrochemical doping

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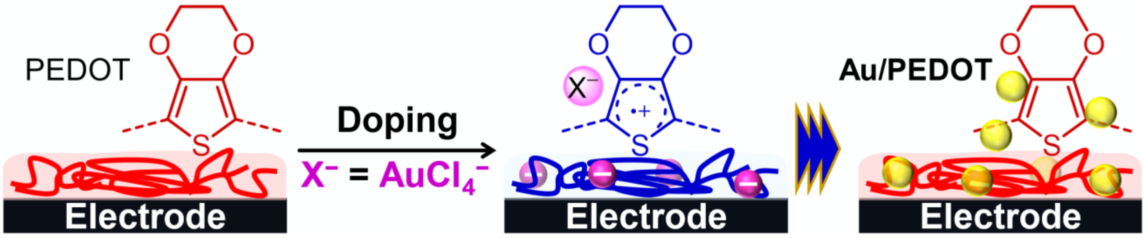
Hybrid materials composed of Au nanoparticles (AuNPs) and conducting polymers (CP) are attractive electrode materials for electrochemical glucose oxidation due to the synergistic properties between Au and CPs. In the hybrid materials, AuNPs serve as catalysts to facilitate the anodic oxidation of glucose, and CPs serve as supporting materials to fix AuNPs on the working electrode. To improve their electrocatalytic properties, the control of the morphologies of AuNPs on CPs is essential.

Here, we demonstrate the electrochemical hybridization of Au with the conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) with the control of the morphologies of Au on PEDOT. The electrochemical hybridization of Au with PEDOT was performed by applying different applied potentials to the PEDOT-coated indium-tin-oxide (ITO) electrode. The Au/PEDOT hybrid material prepared with the application of the potential, where the electrochemical doping of PEDOT and Au electrodeposition simultaneously occurred, showed higher electrocatalytic properties for the electrochemical glucose oxidation than Au/PEDOT hybrid materials prepared under the different applied potentials. The higher electrocatalytic properties were found to be due to the dispersion of AuNPs along the network structures of PEDOT. The Au/PEDOT with the optimal conditions had 12.0 mM of LOD with the linear range from 25 mM to 100 mM.

Keywords: electrochemical hybridization; electrochemical doping; Au nanoparticles; poly(3,4-ethylenedioxythiophene); glucose oxidation



Luminescent lanthanide-containing gelatin/polydextran/laponite nanocomposite hydrogels for sensing applications

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Lanthanide-containing luminescent nanocomposite hydrogels have garnered considerable interest for sensor applications due to their significant Stokes shifts, narrow emission peaks, and prolonged luminescence lifetimes. These hydrogels are frequently utilized for detecting pH variations, small molecules, gases, and volatile organic compounds (VOCs). In this research, we developed several innovative types of lanthanide-containing nanocomposite hydrogels by integrating various lanthanide-embedded laponite (Ln@Lap) into polyethyleneimine-modified gelatin/polydextran aldehyde (PG/PDA) networks through dynamic bonds. We conducted a comprehensive analysis of the structures and properties of these PG/PDA/Ln@Lap nanocomposite hydrogels. The PG/PDA/Ln@Lap hydrogels, characterized by a combination of imine bonds, coordination bonds, hydrogen bonds, and electrostatic interactions, demonstrated exceptional shear-thinning and self-healing properties, making them ideal candidates for electrospinning and 3D printing. In particular, these nanocomposite hydrogels proved to be highly sensitive luminescent sensors for copper(II) (Cu^{2+}) ions and gaseous formaldehyde detection. The luminescent sensors demonstrated an excellent linear relationship in the Cu^{2+} concentration range of 1×10^{-6} to 1×10^{-3} M, with a calculated limit of detection (LOD) of 1.12×10^{-6} M. On the other hand, gaseous formaldehyde was detectable in concentrations from 0.06 to 7.95 ppm, with a calculated LOD of 0.06 ppm. Additionally, these luminescent sensors demonstrated selectivity in competition experiments conducted in the presence of other analytes. Overall, this study introduces a versatile platform of lanthanide-containing nanocomposite hydrogels with dynamic features suitable for both processing and sensing applications.

Keywords: lanthanide; laponite; nanocomposite hydrogels; sensing

Materials Science and Nanotechnology (MN-O-019)

Electrophoretic deposition of nano catalysts on carbon substrates as an enhanced electrode for manganese/iron flow batteries

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Manganese/iron redox flow batteries (Mn/Fe RFBs) can minimize the dependency on critical raw materials like vanadium and reduce the levelized cost of storage of the technology. In spite of this fact, the Mn/Fe RFB is not well studied, which opens an opportunity to develop highly active membrane-electrode-assemblies (MEAs) for this purpose. As a consequence, MXene and carbon nanomaterials (CNMs) that include carbon nanotubes (CNTs) and graphene, along with their nitrogen-doped counterparts (excluding MXene) were decorated on carbon paper and cloth surfaces using electrophoretic deposition (EPD) in this investigation. Prepared electrodes were tested in a three-electrode cell in 0.1 M vanadium sulfate in 1 M sulfuric acid for potential flow battery studies. Cyclic voltammetry and electrochemical impedance spectroscopy were employed to identify the best-performing electrodes, and they were further tested in H-type glass cell studies with Mn/Fe RFB electrolytes. The selected best electrode was evaluated against Nafion 115 using SPEEK (non-fluorinated) cation exchange membranes (CEMs), and the best performing MEA was tested in an Mn/Fe RFB. Additionally, and in parallel, the performance of spray-coated electrodes was also compared to EPD. Comparing the morphological properties of cycled electrodes with pristine counterparts ensured an understating of the MEA's aging mechanism.

Keywords: MXene; CNT; graphene; N-doping; redox flow battery; SPEEK CEM

Materials Science and Nanotechnology (MN-O-020)

Effect of deposition cycles on the catalytic activity of atomic-size gold-modified polyaniline analogues for low alcohol oxidation

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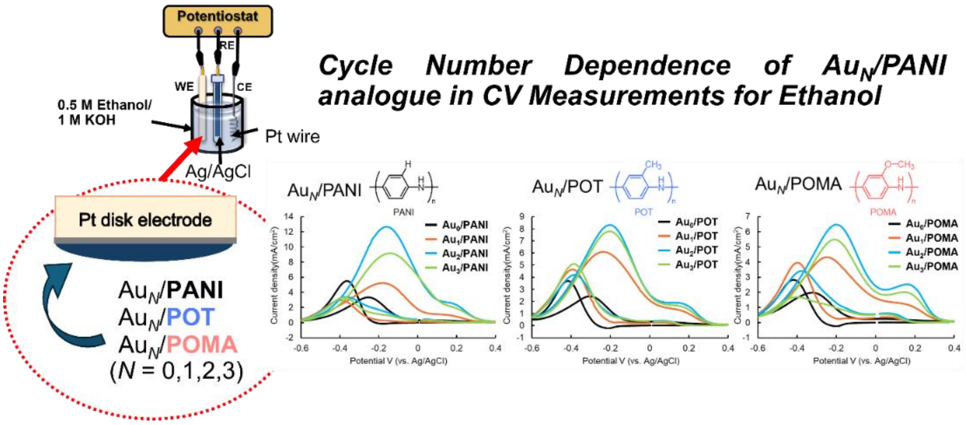
Electrochemical oxidation of low alcohols is widely utilized in sensors and fuel cells using gold (Au) electrocatalysts. Especially, the atomic scale Au electrocatalysts are promising due to their high activity arising from size effects. We have developed the cyclic atomic-sized Au electrodeposition platform using polyaniline (PANI) as a supporting material, discovering their high catalytic activity for alcohol oxidation. Considering the synergistic effects of the hybridization of Au with conductive polymers (CPs) on the electrocatalytic properties, their chemical structures also influence them. On the other hand, the applicable CP to the atomic-sized Au electrodeposition remains limited to PANI.

Here, we expand this limitation to PANI analogue, such as poly(*o*-methoxyaniline) (POMA) and poly(*o*-toluidine) (POT). Various Au_N/PANI analogues, where N represents the number of deposition cycles, are fabricated with the developed the cyclic atomic-sized Au electrodeposition technique, and their electrocatalytic properties are evaluated by cyclic voltammetry (CV) measurements in 1 M KOH (aq) containing lower alcohols.

CV measurements for ethanol gave oxidation current peaks attributed to ethanol oxidation. Regardless of CPs, the observed current was the highest when Au_2/PANI analogue electrodes were used as a working electrode. These results demonstrate the successful electrodeposition of atomic-size Au clusters on PANI analogue.

Keywords: electrochemical oxidation; low alcohol; polyaniline analogue; atomic-size gold; hybrid materials



Materials Science and Nanotechnology (MN-O-023)

Heterocyclic modification leading to luminescent 0D metal organochalcogenide with stable X-ray scintillating properties

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Michael G. Taylor,[2] Worakit Naewtong,[4] Pongsakun Sripetch,[4] Busayakorn Na Ranong,[5]
Tossawat Autila,[5] Thiti Rungseesumran,[5] Jakrapong Kaewkhao,[6] Taweesak Sudyodsuk,[1]
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Metal organochalcogenides (MOCs) are an emerging class of luminescent hybrid organic-inorganic semiconductors whose structures and properties can be tuned by organic functionalization and substitutions of their metal and chalcogen elements. Herein, we present a new design strategy by heterocyclic modification, resulting in the transformation of prototypical two-dimensional (2D) silver phenylselenide (AgSePh) to a zero-dimensional (0D) silver pyridinylselenide (AgSePy) via the formation of Ag-N bonds. At room temperature, AgSePy shows strong and broad orange photoluminescence (PL; λ_{max} = 636 nm, full-width-at-half-maximum = 111 nm, quantum yield = 64%) with a large 259 nm Stoke's shift and a 3.4 μs lifetime. Using steady-state and time-resolved PL spectroscopy under varying temperature and oxygen conditions, we found AgSePy to exhibit air-stable luminescence and maintain a high PL quantum yield and a single exponential PL lifetime down to 4 K. Furthermore, AgSePy shows excellent thermal stability up to ~250 °C and chemical stability against polar, non-polar, and aqueous solvents at pH 3-14. Density functional theory calculations further confirm the 0D electronic structure. Finally, we successfully demonstrated the performance of AgSePy as an X-ray scintillator with an estimated light yield of ~8,000 phe/MeV and a spatial resolution down to 0.080 - 0.005 mm. Overall, this work provides a novel tactic to modify the structures and properties of MOCs, highlighting their structural richness and structure-property relationship, and introduces their new use as X-ray scintillators, encouraging further development in radiation detection and medical imaging.

Keywords: metal organochalcogenides; luminescence; crystals; hybrid organic-inorganic semiconductors; X-ray scintillators

Materials Science and Nanotechnology (MN-O-038)

ESIPT luminophores for high-performance transparent luminescent solar concentrators

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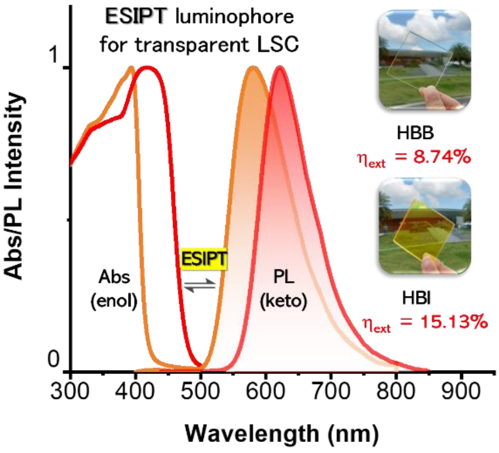
Luminescent solar concentrators (LSCs) hold great potential for building-integrated photovoltaic (BIPV) applications by providing a balance between electricity generation and aesthetic appeal. However, achieving high photoelectric performance in LSCs remains a challenge due to spectral overlap between absorption and emission, leading to self-absorption losses. In this study, we designed and synthesized excited-state intramolecular proton transfer (ESIPT) dyes (namely, **HBB** and **HBI**) embedded in PMMA as a novel class of self-absorption-free luminophores for efficient transparent LSCs. The optimized **HBB** and **HBI**-based LSC slabs exhibited strong keto orange-red emission, benefiting from high-edge photoluminescence quantum yields (42–59%) and a minimal overlap integral (0.30–0.79%). When coupled with silicon solar cells, the luminescent solar concentrator-integrated photovoltaics (LSC-PV) demonstrated high optical efficiency (4.15–9.37%) and a power conversion efficiency of (0.46–1.23%) under AM 1.5G solar illumination. Additionally, a high external quantum efficiency (8.74–15.13%) was achieved, reflecting efficient light harvesting and low optical loss. Notably, the **HBB**-based LSC exhibited an excellent color rendering index (CRI) of 99 and an average visible transmittance (AVT) of 92%. Accordingly, this work paves the way for the development of highly efficient LSCs with reduced self-absorption losses, ultimately enhancing photovoltaic performance and power generation in BIPV applications.

Keywords: luminescent solar concentrator; excited-state intramolecular proton transfer; self-absorption free; organic emitter



Materials Science and Nanotechnology (MN-O-044)

Chelation-free silica sensors for mercury detection and removal

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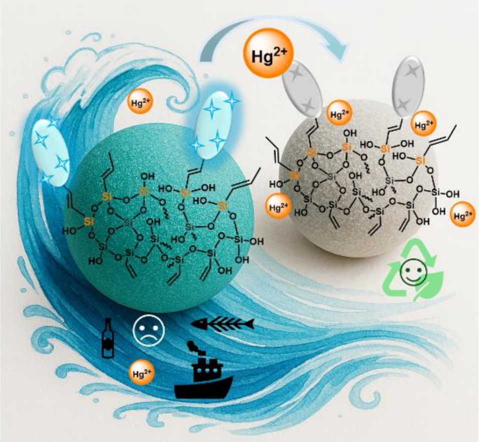
Silica, which constitutes the majority of sand, has recently been recognized as a sustainable material for detecting and eliminating toxic metals such as mercury ions (Hg^{2+}) from soil, groundwater, and industrial pipelines. To address current shortcomings, we identified two environmentally friendly silica-based materials, anthracene-functionalized silica ($AnSiO_2$) and pyrene-functionalized silica ($PySiO_2$), as high-throughput, chelation-free solutions with minimal environmental disruption. Both materials present intense fluorescence in aqueous solutions, especially at pH 6, and strong fluorescence quenching effects, which provide sensitivity for detecting Hg^{2+}. Notably, $PySiO_2$ exhibited the best performance, with a 0.29 μM detection limit and a Stern–Volmer constant of 2×10^6 M^{-1}, together with an outstanding adsorption capacity of 54.04 mg/g, verified by ICP-MS analysis. The sensing mechanism is due to charge–dipole as well as π-electron interactions, substantiated by spectroscopic investigations. Importantly, $PySiO_2$ retains high performance in Hg^{2+} removal after four sorption–desorption cycles and effectively eliminates Hg^{2+} from aquaculture water, indicating its practical applicability. By offering an environmentally friendly approach to remove mercury from exposed areas, these results demonstrate the potential to regulate mercury contamination with inexpensive resources and contribute to sustainable development [*Chem. Asian J.* **2024**, e202401591].

Keywords: silica; mercury ions; fluorescence; chelation-free; environmental remediation



Natural Products, Biological Chemistry and Chemical Biology (NB-O-007)

Lignans and phenolic compounds from the whole plant of *Balanophora fungosa* with DPPH radical scavenging activity and *α*-glucosidase inhibitory activity

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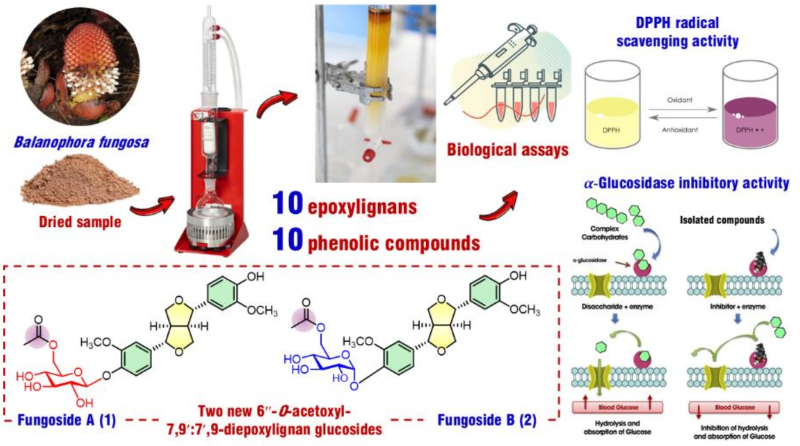
Ten lignans, including two novel 6″-*O*-acetoxyl-7,9′:7′,9-diepoxylignan glucosides, fungoside A (**1**) and fungoside B (**2**), along with eight known ones (**3**–**10**), as well as ten known phenolic compounds (**11**–**20**) were isolated from the whole plant of *Balanophora fungosa*. Their structural elucidation was determined through a comprehensive analysis of NMR spectroscopic and mass spectrometry (MS) data. Notably, compounds **1** and **2**, possess a unique linkage, where the acetyl group is connected to the hydroxymethylene group of *β*-glucose and *α*-glucose moieties, respectively. Regarding DPPH free-radical scavenging activity, lariciresinol (**7**) displayed strong activity with an IC_{50} value of 10.9 µM, similar to that of trolox, a positive control (IC_{50}, 8.2 µM). In terms of *α*-glucosidase inhibitory activity, dihydrosesamin (**8**) had the strongest inhibition against *α*-glucosidase with an IC_{50} value of 9.1 µM, stronger than that of a positive control, acarbose (IC_{50}, 185.2 µM). This study is the first to identify these compounds and evaluate their *α*-glucosidase inhibitory activity. The results indicate that the traditional use of this species in Vietnamese folk medicine for diabetes management may be attributed to the *α*-glucosidase inhibitory properties of its constituents.

Keywords: 7,9′:7′,9-diepoxylignan glucosides; *Balanophora fungosa*; Balanophoraceae; *α*-glucosidase inhibitory activity; free-radical scavenging



Natural Products, Biological Chemistry and Chemical Biology (NB-O-010)

Semi-synthesis and biological evaluation of dimethylcardamonin (DMC) derivatives as a potential agent against cervical cancer cells

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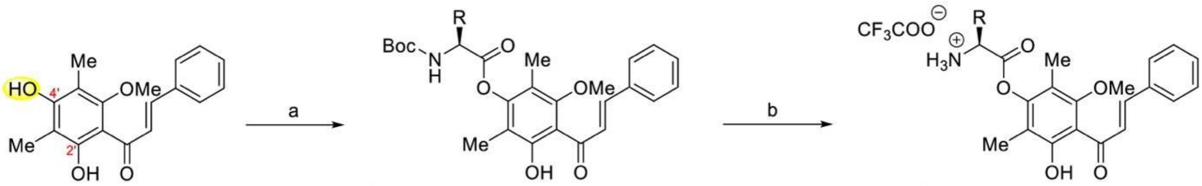
Chemical structure of 2′,4′-dihydroxy-6′-methoxy-3′,5′-dimethylchalcone (DMC, **1**), a phytochemical from *Syzygium nervosum* seeds, was modified in order to improve its anticancer activity and water solubility by conjugating with two amino acids, L-alanine and L-valine, to afford the DMC derivatives **3a** and **3b** *via* the intermediates **2a** and **2b**, respectively. Compounds **3a** and **3b** demonstrated notable antiproliferative effects in a cervical cancer cell line (SiHa). The IC_{50} values were 7.56 ± 0.27 µM (**3a**) and 8.24 ± 0.14 µM (**3b**), approximately twice as effective as compound **1**. Wound healing assays, cell cycle studies, and mRNA expression analyses were performed to investigate its mechanisms. Both compounds inhibited SiHa cell migration and caused cell cycle arrest at the G1 phase. Compound **3a** exhibited strong anticancer potential by upregulating *TP53* and *CDKN1A*, which led to elevated *BAX* levels and reduced expressions of *CDK2* and *BCL2*, promoting apoptosis *via* intrinsic pathways. The *BAX*/*BCL2* ratio increased significantly post-treatment, confirming its pro-apoptotic effects. *In silico* molecular dynamics simulations and binding energy calculations revealed interactions between compound **3a**, **3b** and HPV16 E6, a cervical cancer-associated oncoprotein. These findings highlight compound **3a** as a promising candidate for anti-cervical cancer drug development due to its enhanced biological activities and mechanistic efficacy.

Keywords: anti-cervical cancer; 4′-O-(L-alanylated) DMC; cell G0/G1 phase cycle arrest; apoptosis; *BAX*/*BCL2* ratio



DMC (**1**)

4′-*O*-(*N*-Boc-L-aminoacylated) DMC (**2**)

2a: R = CH_3 (Alanine)
2b: R = $CH(CH_3)_2$ (Valine)

4′-*O*-(L-aminoacylated) DMC (**3**)

3a: R = CH_3 (Alanine)
3b: R = $CH(CH_3)_2$ (Valine)

Natural Products, Biological Chemistry and Chemical Biology (NB-O-036)

Peptidyl liposome for trigger-responsive liposomal delivery

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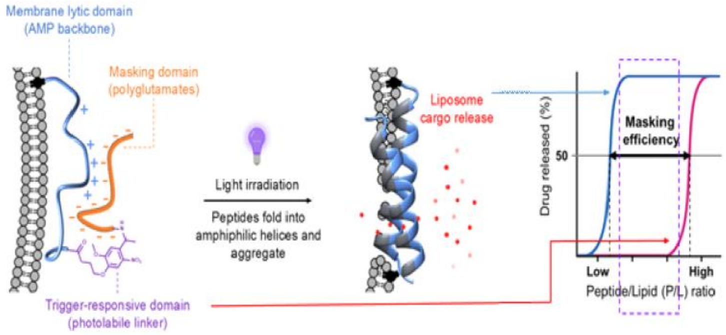
The quest to develop "smart" peptidyl liposomes that can respond to specific stimuli has seen numerous efforts. However, the outcomes of these endeavors have been limited. In this study, we challenge the conventional understanding of binary peptide-membrane interactions (peptide-membrane interaction without conjugation) and propose a novel approach by examining peptide-membrane interactions in a unary manner (conjugation of peptides and membranes). We have discovered that an antimicrobial peptide previously considered inert to zwitterionic membranes (common in therapeutic liposomes) is an excellent membrane lytic backbone for smart peptidyl liposomes. Our developed peptidyl liposome demonstrates exceptional stability during the signal-waiting phase and successfully releases upon triggering. Building on this breakthrough, we are currently developing additional trigger-responsive peptidyl liposomes capable of responding to disease-associated enzymes. These findings offer new perspectives and opportunities in the realm of advanced drug delivery systems.

Keywords: liposome; peptide; triggered-release; controlled-release



Organic Synthesis and Medicinal Chemistry (OM-O-005)

From agricultural by-products to bioactive compounds: The potential of immature pomelo peels (IPPs) in medicinal chemistry

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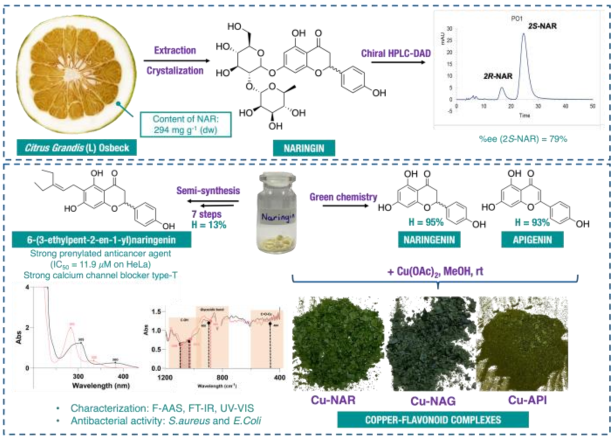
The exploitation of agricultural by-products has been emerging, particularly in the fields of medicinal chemistry, drug screening, and sustainable development. In particular, the immature pomelo peels (IPPs) from Tien Giang Province, Vietnam, have been studied for their ability to isolate naringin, which serves as a precursor for the semi-synthesis of various bioactive compounds, including naringenin, apigenin, flavonoid-metal complexes, and the prenylatedflavanone (6-PFVN) as an anticancer agent and efficiency calcium channel blocker in neuropathic pain relief. With a high naringin isolation yield and an enantiomeric excess (%*ee*) of 79% for the 2*S*-naringin isomer, the green semi-synthesis of apigenin from naringin was successfully conducted using I_2/DMSO-H_2O catalyst. Additionally, naringenin, an aglycone derived from naringin with diverse biological activities, was also synthesized and subsequently used to prepare 6-PFVN through a seven-step semi-synthesis process which yielded 13%. Moreover, the synthesis of flavonoid-metal complexes from naringin, naringenin, and apigenin has demonstrated promising results, highlighting their potential in enhanced bioactivity of antibacterial. The final product, 6-(3-ethylpent-2-en-1-yl)-naringenin (6-PFVN), has been shown to exhibit potent anti-cancer activity against cervical cancer cells, with an IC_{50} of 11 μM, and demonstrates compatibility with docking processes on the ERα receptor. These studies provide compelling evidence of the economic and medicinal potential of this agricultural by-product, paving the way for sustainable applications in drug development.

Keywords: immature pomelo peels; naringin; naringenin; apigenin; anti-cancer; prenylated flavanone; antibacterial



Organic Synthesis and Medicinal Chemistry (OM-O-009)

Total synthesis of lobatamides

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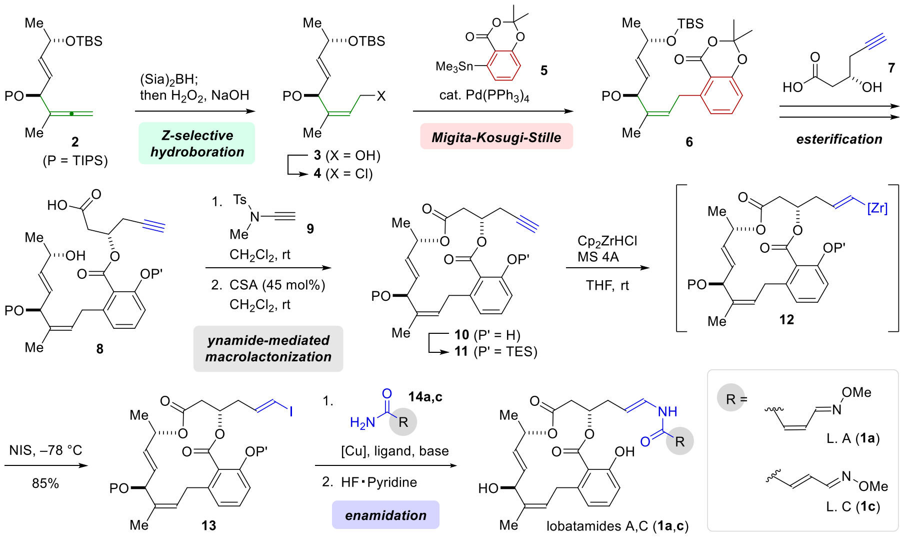
Lobatamides A-C (**1a**–**c**), isolated from a southwestern Pacific tunicate by Boyd and Suzumura, are expected as a new class of antitumor agents through V-ATPase inhibition. Structurally, they share a common macrobislactone framework with various enamide side chains. These enamide side chains are known to be crucial for their biological activity, although the details of the systematic structure-activity relationship are not investigated. In this presentation, we report the total synthesis of lobatamides A (**1a**) and C (**1c**) based on the stereoselective construction of the *Z*-allylic arene moiety, and the late-stage installation of the enamide side chains from the terminal alkyne.

The *Z*-selective hydroboration of 1,1-disubstituted allene **2** and subsequent Migita-Kosugi-Stille coupling provided (*Z*)-allylic arene moiety **6**. Macrobislactone framework **11** was synthesized through intermolecular esterification with **7** and ynamide-mediated macrolactonization. The salient feature of our synthesis was the late-stage installation of enamide side chains from common intermediate **11**. Treatment of **11** with the Schwartz reagent [Cp_2ZrHCl] promoted hydrozirconation to afford (*E*)-vinylic intermediate **12** without affecting the macrobislactone core. Subsequent iodination with NIS provided (*E*)-vinylic iodide **13**. Finally, the copper-mediated enamidation with **14a** and **14c**, and the deprotection accomplished the total synthesis of lobatamides A (**1a**) and C (**1c**) [*ACIE.* **2024**, *63*, e202402335].

Keywords: enamide; hydroboration; macrolactonization; Schwartz's reagent; total synthesis



Organic Synthesis and Medicinal Chemistry (OM-O-011)

Multifunctional molecular hybrid composed of doxorubicin, AS1411 aptamer, and T9/U4 ASO for targeting colorectal cancer cells

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Colorectal cancer (CRC) is a major global health concern, including in Thailand, where current treatments often lack specificity and efficiency. To address these limitations, a multifunctional drug delivery platform has been developed, combining bioactive materials with targeted ligands. Aptamers, short synthetic DNA or RNA sequences, are used as binding ligands due to their high specificity for target molecules, making them ideal for cancer therapy. Additionally, antisense oligonucleotides (ASOs) disrupt transcription processes, silencing target mRNA pathways. This study focused on creating a drug delivery system using the AS1411 aptamer, T9/U4 ASO, and doxorubicin to regulate SW480 cancer cell proliferation. The AS1411 aptamer targets nucleolin, overexpressed on cancer cells, while T9/U4 ASO inhibits human telomerase RNA, preventing cancer growth. The molecular hybrid was prepared through oligonucleotide hybridization and loaded with doxorubicin. Characterization using fluorescence microscopy and flow cytometry confirmed its specific recognition of SW480 cells and antiproliferative effects. Importantly, the system showed lower toxicity in normal cells. These findings suggest the platform's potential for incorporating other chemotherapeutic drugs and bioactive materials to improve cancer treatment efficacy.

Keywords: AS1411 aptamer; antisense oligonucleotide; doxorubicin; colorectal cancer

Organic Synthesis and Medicinal Chemistry (OM-O-013)

Coupling reactions in water using palladium catalysts covalently tethered on a thermo-responsive polymer

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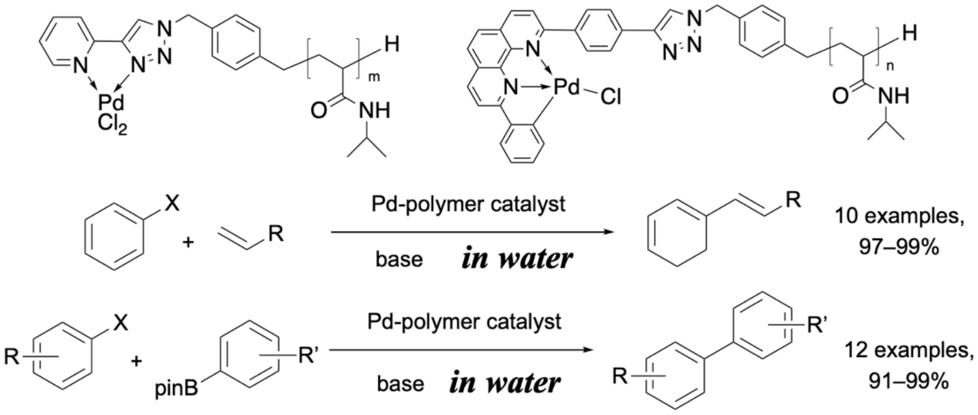
In the manufacturing process of organic chemicals, replacing the organic solvents with water is an important issue from the viewpoint of sustainable technology. In this study, we report on a method to carry out organic reactions in water by using catalysts immobilized on thermo-responsive polymers. Bidentate N,N-ligands were covalently tethered on a reversible addition-fragmentation chain transfer (RAFT) agent, and poly(*N*-isopropylacrylamide) (PNIPAAm) bearing those ligand moiety was prepared by living-radical polymerization using these RAFT agents. Then, a palladium complex covalently immobilized at the terminus of each polymer chain was synthesized. Palladium-catalyzed Mizoroki-Heck and Suzuki-Miyaura cross coupling reactions proceeded in water with these polymer-tethered Pd catalysts. The products were obtained by easy extraction with ethyl acetate in good yields with 0.01 mol% Pd loading and the aqueous layer containing the polymer catalysts could be reused. Thanks to the thermo-responsive segment, the polymer-tethered catalyst joined the reaction during heating and dissolved in water after the reaction by cooling. This allowed easier extraction of the product. Electron microscopic analysis suggested that palladium nanoparticles formed during the reaction were responsible for the catalytic activity. The aqueous solution could be reused 8 times, and a turnover number (TON) of up to 82,800.

Keywords: palladium; catalyst; reaction in water; thermo-responsive polymer; poly(*N*-isopropylacrylamide)



Organic Synthesis and Medicinal Chemistry (OM-O-017)

Skeletal editing of benzimidazole-based NHCs to quinoxalines by carbon atom insertion

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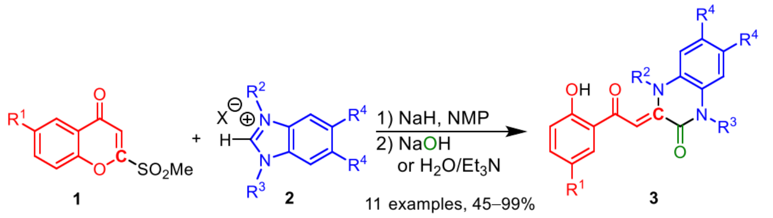
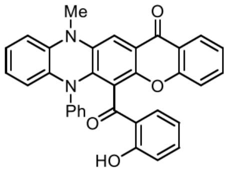
While skeletal editing has the potential to simplify synthetic strategies for natural products and to accelerate drug discovery, viable methodologies applicable to various substrates remain limited. As another method for skeletal editing, we present a new carbon atom insertion reaction of benzimidazole-based *N*-heterocyclic carbenes (NHCs) to 3-methylene-3,4-dihydroquinoxalin-2(1H)-ones **3**, a scaffold found in numbers of bioactive compounds. When benzimidazoliums **2** were reacted with 2-(methylsulfonyl)chromones **1** under basic conditions, followed by the treatment with a basic aqueous solution/mixture, the carbon atoms located at position **2** of the chromones were inserted into the in situ-generated NHCs from **2** to afford quinoxalinones **3**. Under the same conditions, 1-methyl-3-phenylbenzimidazolium iodide (**2** with R^2 = Me, R^3 = Ph, R^4 = H) provided an unexpected pentacyclic product **4** in an excellent yield presumably via a pathway involving an annulation with a single-carbon unit originating either from the NHC or N-methyl-2-pyrrolidone (NMP) used as a solvent. This transformation allows for the efficient synthesis of highly substituted quinoxalinones in one pot from simple starting materials.

Keywords: NHC; benzimidazole; quinoxaline; skeletal editing; carbon atom insertion





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Organic Synthesis and Medicinal Chemistry (OM-O-021)

Synthesis of natural and unnatural products through selective coupling

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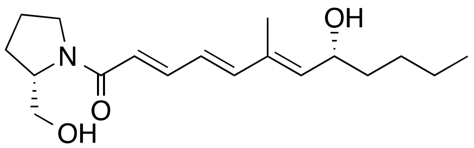
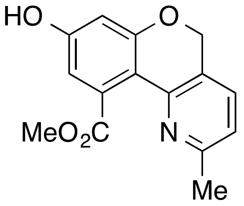
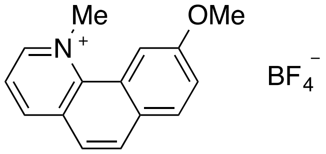
Coupling reactions are in indispensable tool in organic synthesis, being especially suited to forming bonds between aryl, vinyl and alkynyl moieties. Amongst natural products, we have achieved the synthesis of viriditins A and B using selective coupling reactions of 1,2-dichloroethylene. This employed sequential Suzuki and Heck reactions. Based upon DFT calculations, we can explain the selectivity in terms of transition state stabilisation by the inductive effect of additional electronegative atoms. In addition, we have completed the synthesis of phochrodines A, B and C utilizing CH-activation chemistry to achieve biaryl coupling, followed by catalytic carbonylation. The synthesis of unnatural products is also important. We have developed a flexible synthesis of donor-acceptor substituted phenanthrenes and aza-phenathrenes based upon CH activation. The photophysicial properties of these compounds have been studied. The extension of this chemistry to the synthesis of picenes will also be discussed.

Keywords: coupling; triene; natural product; CH activation; phenanthrene







Organic Synthesis and Medicinal Chemistry (OM-O-034)

On-water accelerated sulfenylation of indole derivatives under visible-light irradiation

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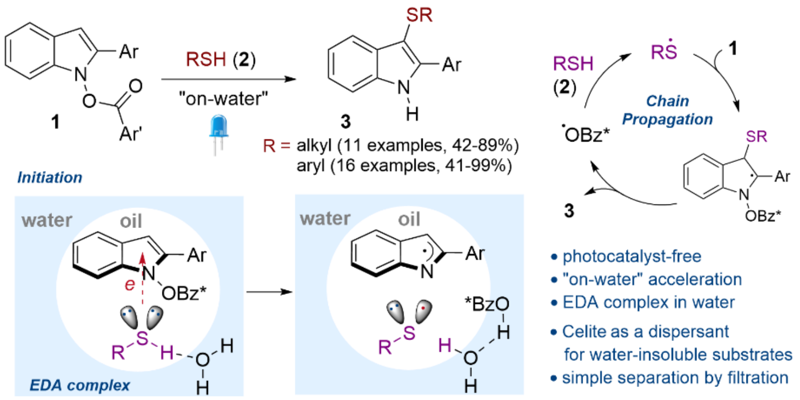
A visible-light promoted sulfenylation of N-acyloxyindole derivatives with thiols has been developed for the synthesis of 3-sulfenylindoles. The reaction exhibits remarkable acceleration in water, whereas the reactions in a homogeneous organic phase were slower and less selective. Water-insoluble reactants often formed aggregates in water leading to low conversion, which can be mitigated by adding Celite as a dispersant. It is proposed that the water-oil interface facilitates EDA complex formation, enhancing single electron transfer (SET) and proton transfer (PT) to generate a thiyl radical. The process is applicable to the synthesis of tubulin polymerase inhibitors, and the product can be conveniently isolated by simple filtration. This study underscores the promising potential of using on-water conditions for advancing future photocatalytic reactions.

Keywords: on-water; photochemical reaction; EDA (electron donor-acceptor) complex; radical chain; thiyl radical



Organic Synthesis and Medicinal Chemistry (OM-O-038)

Molecular reconstruction with stereochemical relay: An investigation into the rearrangement of spiro[4.5]decadienone to benzoxepane

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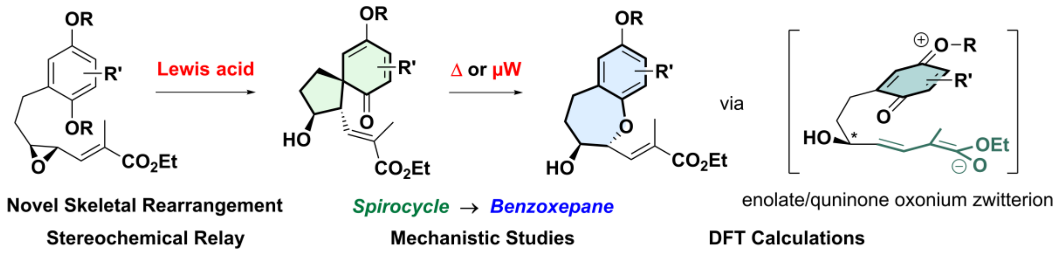
Herein, we report the unusual skeletal rearrangement of spiro[4.5]decadienone to benzoxepane. In particular, Lewis acid-promoted epoxide-opening *ipso*-cyclization of aryl epoxides afforded spiro[4.5]decadienone intermediates. Subsequent thermal activation assembled a benzoxepane core via rearomative molecular reorganization. The sequence was high-yielding and highly diastereoselective but sensitive to the aromatic substitution pattern and the epoxide side chain. Mechanistic studies suggested that the rearrangement proceeded via an uncommon intramolecular enolate attack onto the electrophilic *O* of *p*-quinone oxonium zwitterion. DFT calculations helped rationalize the product distribution and the origin of diastereoselectivity. Initial investigation into the application of this chemical transformation is also presented. [*Chem. Asian J.* **2024**, *19*, e202300937.]

Keywords: rearrangement; spiro compounds; benzoxepane; stereochemical relay



Organic Synthesis and Medicinal Chemistry (OM-O-042)

Total synthesis of tilivalline

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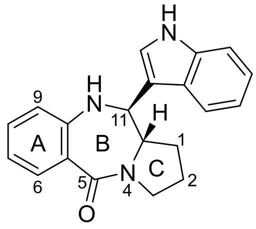
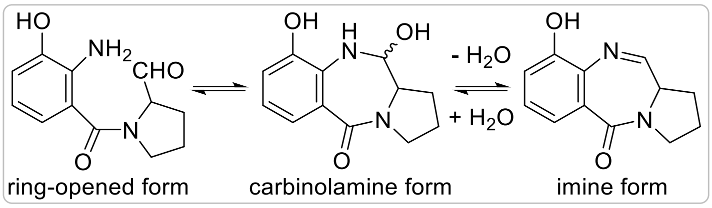
Tilivalline (**1**) is a C11-indol-3-yl-substituted pyrrolo[2,1-*c*][l,4]benzodiazepine (PBD) metabolite isolated from *Klebsiella pneumoniae var. oxytoca* by Mohr and Budzikiewicz in 1982 [*Tetrahedron* **1982**, *38*, 147]. Tilivalline (**1**) displayed growth-inhibitory activity against leukemia L1210 cells and was identified as a potential pathogenic factor linked to antibiotic associated hemorrhagic colitis (AAHC) caused by overgrowth of inherently β-lactamase resistant *K. oxytoca* in colon. The biosynthetic studies suggested that the PBD core structure was assembled *via* nonribosomal peptide synthetase (NRPS) from 3-hydroxyanthranilic acid and proline [*Angew. Chem. Int. Ed.* **2017**, *56*, 14753]. Nevertheless, the incorporation of the indole moiety is resulted from non-enzymatic spontaneous Friedel-Crafts type reaction of the PBD precursor, tilimycin (**2**), with biogenetically generated indole to furnish the formation of tilivalline (**1**). Coincidently, the chemical synthesis of tilivalline (**1**) in literature mostly employed the similar approach as the biosynthesis in Nature. Previous synthesis focused on the construction of the PBD core structure followed by the incorporation of the indol-3-yl substituent by Friedel-Crafts alkylation reaction at C11 of PBD precursors. The late stage electrophilic aromatic substitution (EAS) reaction gives rise to the stereoselective issue and restricts the C11-substituent to exceptionally π-electron rich (het)aryl groups. The emerging new biological activities of tilivalline (**1**) and the paucity of C11-aryl PBDs have prompted us to investigate a general strategy for the total synthesis of tilivalline (**1**) and other C11-aryl PBD analogs. The synthesis of tilivalline started with l-proline as the C-ring component. After converting the carboxylic acid to an aldehyde group, a stereoselective addition reaction of indol-3-yl-Grignard reagent guided by the α-chiral center (C11a) was carried out to establish the stereocenter at C11. Meanwhile, the amide bond formation between the Grignard reaction adduct with *o*-aminobenzoic acid was accomplished to introduce the C-ring counterpart. The final cyclization of the PBD skeleton was constructed using a stereoselective acid-catalyzed dehydration cyclization approach (between N10-C11). We anticipate that this work would open up a new opportunity for the remaining unexplored medicinal chemical space of PBDs.

Keywords: pyrrolo[2,1-*c*][l,4]benzodiazepine; PBD; tilivalline; tilimycin



tilivalline (**1**)



kleboxymycin (tilimycin, **2**)

Organic Synthesis and Medicinal Chemistry (OM-O-047)

Facile on-bead amidation for the synthesis of cyclic peptides

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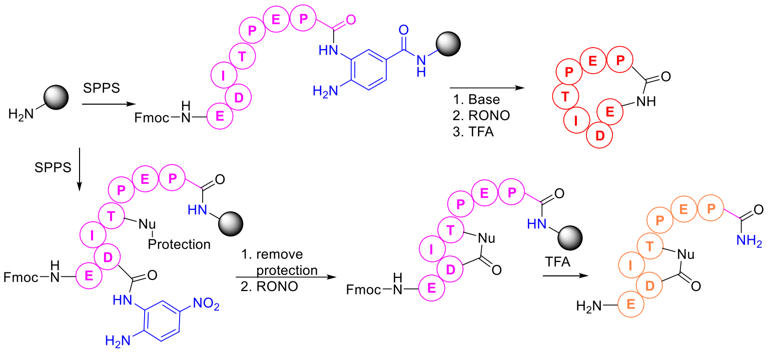
Cyclic peptides are one of the peptides that exist in nature. Besides, the cyclization strategy is a popular way to improve the pharmaceutical properties of linear therapeutical peptides. Despite its significant role, the synthesis of cyclic peptides remains challenging in peptide synthesis. The conventional approach cyclized the linear peptides in the solution with low concentration to prevent dimerization. However, it causes a slow reaction and generates side reactions, eventually leading to laborious purification and low yields. Herein, we reported a diaminobenzoate resin for the on-bead cyclization to generate head-to-tail cyclic peptides. Furthermore, 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. Upon activation by nitrite, the following acylbenzotriazole is a leaving group for the on-bead cyclization for the formation of tail-to-side chain and side chain-to-side chain cyclic peptides.

Keywords: solid-phase peptide synthesis; on-bead cyclization; diaminonitrobenzene; benzotriazole; cyclic amide



Advantages: Fast reaction, Less purifiction effort, moderate to high yield.

Organic Synthesis and Medicinal Chemistry (OM-O-055)

Supramolecular assemblies of porphyrin derivatives for their functional applications

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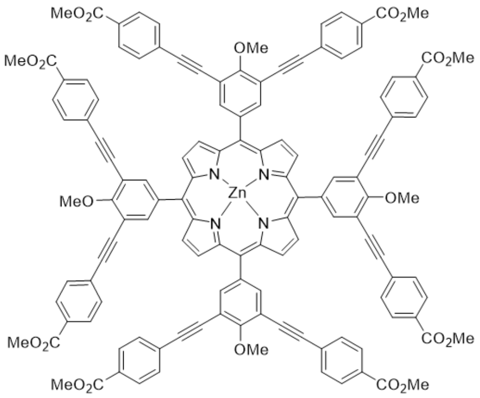
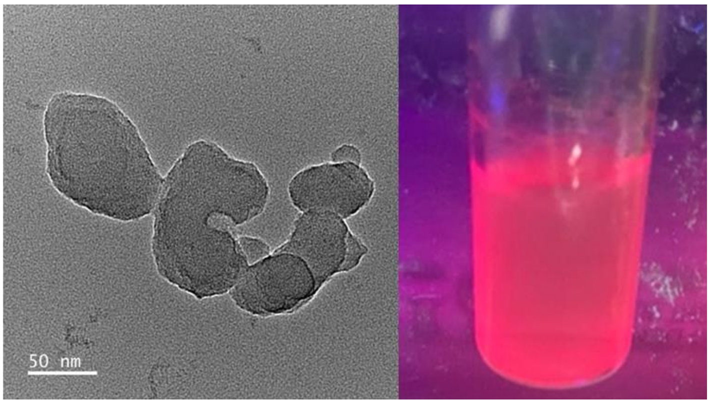
Porphyrin derivatives have been widely employed in photodynamic therapy (PDT), optoelectronic devices, and catalysis due to their unique photochemical and photophysical properties. In recent years, supramolecular assemblies of porphyrins have emerged as promising platforms for developing photo-responsive smart materials, energy conversion systems, and functional biomaterials. In this study, we synthesized a series of porphyrin-based molecules capable of forming self-assembled structures. A porphyrin dendrimer exhibiting efficient light-harvesting and energy transfer properties was used to construct coordination-driven supramolecular polymers. Additionally, multi-pyridyl porphyrin derivatives were designed to facilitate metal-ligand coordination. These porphyrins demonstrated a strong ability to generate reactive oxygen species (ROS) upon light irradiation and ultrasound exposure, highlighting their potential as dual-activated agents for photodynamic and sonodynamic cancer therapy.

Keywords: supramolecular assembly; porphyrin; PDT





Organic Synthesis and Medicinal Chemistry (OM-O-058)

Unexpected six-membered ring formation during *in-situ* halogenation of scortechinone D using oxone and sodium halide

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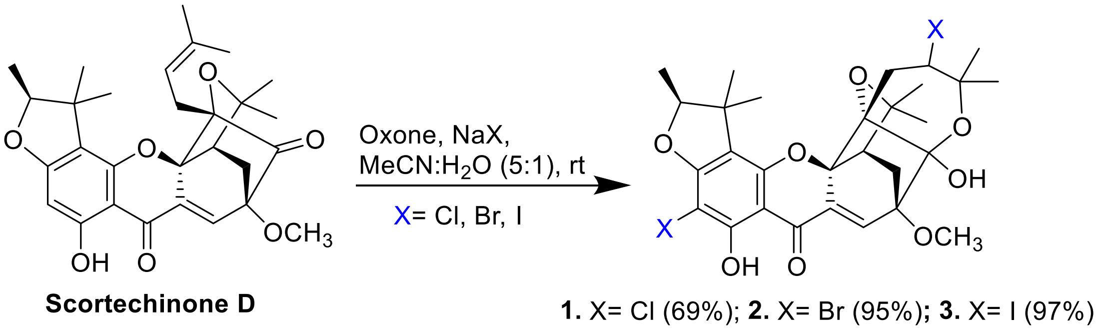
Scortechinone D, a type of secondary metabolite of cage xanthone, is inclusively found in the Garcinia genus. These compounds not only possess distinctive structures but also exhibit intriguing biological properties, including cytotoxic, anti-inflammatory, and antimicrobial effects. The incorporation of halogens, including chlorine, bromine, and iodine, into organic molecules has been extensively investigated for its impact on pharmacological properties and biomedical applications. Thus, this study aims to initiate synthesis of halogenated scortechinone D via *in-situ* halogenation using oxone® and sodium halide in MeCN:H_2O (5:1) at ambient temperature. The result shows that halogenation attacks not only on aromatic ring, but also the formation of six-membered ring occurs via halo-hydroxylation of isoprenyl followed by attacking of hydroxyl to carbonyl to form tetrahydropyran ring with moderate to good yield.

Keywords: cage xanthone; garcinia; halogenation; oxone; scortechinone D



1. X= Cl (69%); **2.** X= Br (95%); **3.** X= I (97%)

Organic Synthesis and Medicinal Chemistry (OM-O-059)

Molybdenum-catalyzed metathesis dimerization/desymmetrization of C_s-symmetric divinylferrocenes

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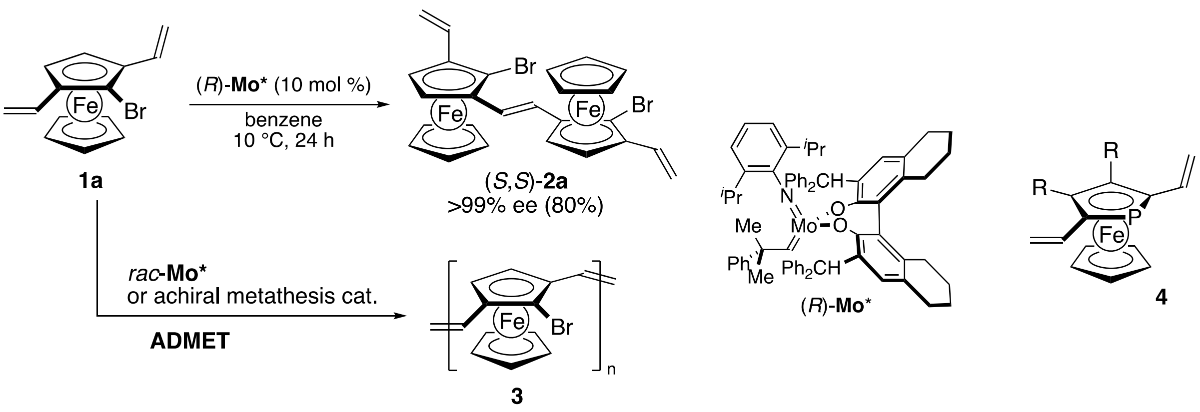
In the last few decades, we have been interested in modulating transition-metal complexes by the ring-closing metathesis (RCM) reaction. The RCM strategies have been successfully extended to the enantioselective counterparts by the use of a chiral molybdenum-alkylidene catalyst producing various planar-chiral complexes (*Chem. Rec.* **2021**, *21*, 3509). Very recently, we reported a novel mode of the asymmetric olefin metathesis reaction, that is *the asymmetric metathesis dimerization (AMD)/kinetic resolution* of racemic planar-chiral vinylferrocene derivatives (*Org. Lett.* **2022**, *24*, 7355; *Organometallics* **2023**, *42*, 1629). Here, we report an enantioselective desymmetrization variant of the AMD method starting with C_s-symmetric divinylferrocene substrates **1**. The AMD/desymmetrization of 2-bromo-1,3-divinylferrocene **1a** was promoted by chiral Mo-alkylidene catalyst (*R*)-**Mo*** to give the corresponding planar-chiral bisferrocene derivative (*S*,*S*)-**2a** of >99% ee in 80% yield. (*R*)-**Mo*** catalyst effectively discriminates the two planar-enantiotopic vinyl groups in **1a** to realize the highly enantioselective reaction. On the other hand, a non-enantioselective reaction of **1a** by *rac*-**Mo*** or achiral metathesis catalysts provided oligomeric/polymeric **3** via ADMET process. The AMD/desymmetrization could be applicable to divinylphosphaferrocene substrates **4** as well. Scope of the AMD/desymmetrization protocol will be presented in detail.

Keywords: ferrocene; planar-chiral; olefin metathesis; desymmetrization; molybdenum



Polymers and Bio-based Materials (PC-O-003)

Optimizing superabsorbent hydrogel-biochar composites synthesis as efficient water-retention agent

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Agriculture sector is facing many challenges, such as climate change, sustainable natural resources management, water shortage and runoff losses. The development of agronomic strategies to mitigate the adverse impact of water shortage crisis due to drought stress is of high priority. Superabsorbent hydrogels can be used as soil amendment in improving water holding capacity and plant available water in soils. Superabsorbent hydrogel-biochar composites (DNHBCR*x*) containing palm kernel shell biochar (BC), potassium poly(acrylate-*co*-acrylamide) and poly(vinyl alcohol) (PVA) were fabricated in a two-step reaction: free-radical random copolymerization and cyclic freeze-thaw. Equilibrium water absorption of the synthesized DHNBCR*x* hydrogels were thoroughly investigated by optimizing various synthetic parameters via Response Surface Methodology-Central Composite Design (RSM-CCD): concentrations of methylene bisacrylamide (MBA) crosslinker, PVA and BC. From 17 experimental runs, the DNHBCR*x* hydrogels showed deionized (DI) water absorption ranging between 44–480 g/g. The DNHBCR1 and DNHBCR7 compositions exhibited superior structural integrity in swollen state and excellent DI water absorption (309–330 g/g), which are recommended as water-retention agents of higher structural durability in the soils. Our findings indicate that the superabsorbent DNHBCR*x* with optimized water absorption properties are a potential candidate to be developed as multifunctional controlled-release applications.

Keywords: hydrogel-biochar composite; optimization; response surface methodology-central composite design (RSM-CCD); water absorption

Polymers and Bio-based Materials (PC-O-005)

Novel endolysin treatment with PVA produced by electrospinning for potential antibacterial

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Bacteriophages are natural bacterial predators that lyse host cells using endolysins, enzymes that rapidly degrade the peptidoglycan layer. This targeted action makes endolysins a promising eco-friendly alternative to antibiotics against resistant bacteria. Poly(vinyl alcohol) (PVA), a biocompatible and stable polymer, is widely used across industries. Electrospun PVA fibers, with high porosity and surface area, provide an ideal platform for endolysin immobilization, preserving activity while enabling efficient recovery for antibacterial applications. In this study, endolysin genes were extracted from two novel phages: Phage C-a, which carries a single endolysin gene, and Phage ECF5_01, which possesses two distinct genes, ORF052 and ORF115. These genes were cloned, expressed in *E. coli* BL21, and immobilized onto electrospun PVA fibers, forming micro- to nano-scale membranes now undergoing antibacterial testing. Despite significant progress, challenges remain in optimizing expression and application. Overcoming these hurdles will advance strategies against antibiotic resistance, with major implications for chemistry and medicine.

Keywords: bacteriophage; endolysin; PVA nanofiber

Polymers and Bio-based Materials (PC-O-006)

Structure regulation of polydextran-based hydrogel by monk fruit saponin: Surmount the dilemma between the stability of hydrogel and bacteriophage release

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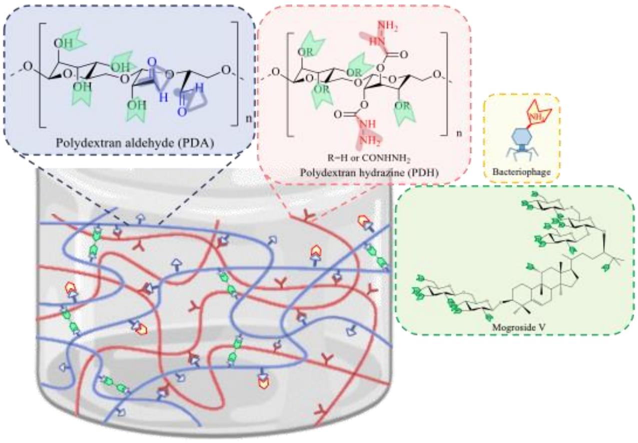
The stability of hydrogel for proper bacteriophage release and its' effect on bacteriophage activity has not been discussed thoroughly. We hypothesized that amphiphilic molecules interact with hydrophilic hydrogel to stabilize hydrogel structure while disrupting the hydrophobic bacterial outer membrane to sensitize the bacteria for easier phage infection when they are released. This study used hydrogel composed of polydextran aldehyde (PDA) and polydextran hydrazine (PDH) for phage delivery. Introducing mogroside V, an amphiphilic substance, into PDA/PDH hydrogels transformed the microstructures with an increased pore area while doubling the compression stress simultaneously. Mogroside V has a hydrophobic aglycone center and five hydrophilic peripheral glucose moieties linked via glycosidic bonds. This property helps mogroside V interact with PDA/PDH hydrogels through hydrogen and hemiacetal bonds to strengthen hydrogel structure, which is partially disrupted when submerged and incubated in water. A synchronized phage and mogroside V release profile showed two asymmetrical release peaks. mogroside V improved the phage's infection rate to 68% on *Escherichia coli* (*E. coli*) after 24 h of incubation, which was 27% higher than the non-mogroside V phage delivery system. The system exerts no cytotoxic effect on mouse embryonic fibroblasts. Integrating mogroside V and phage into hydrogel introduces a novel antibacterial system that avoids the risk of antibiotic-resistant bacteria development.

Keywords: bacteriophage; polydextran; mogroside V



Polymers and Bio-based Materials (PC-O-008)

One ppm-detectable hydrogen gas sensor based on nanostructured polyaniline

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Munziya Abutalip,[2] Bakhtiyar Soltabayev,[3] Amanzhol Turlybekuly,[3] Salimgerey Adilov,[4]
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The hydrogen (H_2) energy industry has continued to expand in recent years due to the decarbonization of the global energy system and the drive for sustainable development. Due to the high flammability of hydrogen and significant safety risks, effective hydrogen detection is becoming an increasingly pressing issue today. Recent studies indicated that the heterostructure design of polyaniline composite materials is an important strategy to enhance gas sensing performance through increasing the carrier mobility. We fabricated hollow tubular and film nanostructures of polyaniline inspired by tubular structure (like CNT) and 2D-nanomaterials (like graphene) and tested obtained materials for the hydrogen sensing performance in parallel with short nanofibers via studying the hole mobility and carrier concentration. In this work, a new type of relatively fast and responsive conducting polymer sensor has been demonstrated for tracing H_2 gas in a nitrogen environment. Three different PANI sensors consisting of hollow tube, film and short nanofiber were evaluated for hydrogen sensing. Among them, the PANI hollow nanotubes exhibited excellent detection performance compared to the thin film sensors and obtained a response of 29% in the experimental data, with a response time of 15 s, which has better performance than PANI thin film (20%). The sensing performance of the hollow tubes were directly proportional to their carrier mobility and carrier concentration. In addition, the hollow nanotube structure of polyaniline provided the best conductivity (9.15 S/cm), followed by PANI thin film (0.60 S/cm) and PANI nanofiber (0.05 S/cm). This conducting polymer-based hydrogen sensor holds promise for the early detection of H_2 leaks in a wide range of industries.

Keywords: conducting polymers; polyaniline; hydrogen sensing; polymer nanostructures

Polymers and Bio-based Materials (PC-O-011)

Stimuli-responsive fluorochromic polymer nanoparticles with polycyclic aromatic backbone

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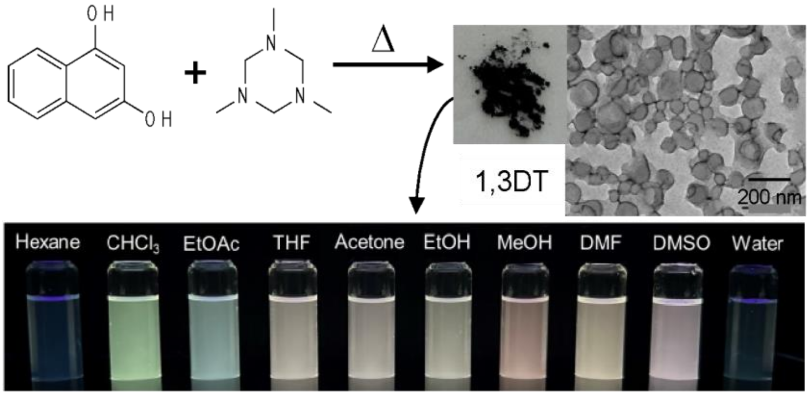
Fluorescent nanoparticles have been widely used in various fields, such as fluorescence imaging and cell labelling. Due to the flexible structural design of main chain and functional groups, polymer-based luminescent materials can provide a versatile platform to realize color-tunable fluorescent particles. We have reported that precipitation polymerization of phenolic molecules with cyclic amines as crosslinker yields spherical polymer microparticles to which polycyclic aromatic moieties can be introduced into the polymer backbone by using various phenolic monomers. In this report, we describe the synthesis of polycyclic aromatic polymer nanoparticles using various polycyclic phenols and their luminescence behavior including solvatochromic properties. For instance, polymer nanoparticles could be obtained by precipitation polymerization of 1,3-dihydroxynaphthalene and 1,3,5-trimethyl-1,3,5-triazinane as a crosslinker. The emission color of the obtained particles (1,3DT, 120 nm) were obviously depends on the type of solvent, e.g. green-yellow in chloroform and red in DMSO. Fluorescent spectra showed emission peaks at 490 and 640 nm in chloroform, and 441 and 650 nm in DMSO respectively with different intensity ratios of the emission peaks. The emission color could be easily controlled by varying the phenol monomer and the polymer network structure inside the nanoparticles, and was also responsive to additives such as metal ion.

Keywords: naphthoxazine polymer; spherical nanoparticles; mono-disperse; fluorescence



under UV light (365 nm)

Polymers and Bio-based Materials (PC-O-013)

A woody composite from arylated lignin and cellulose via one-step fractionation

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As the second most abundant biopolymer resource in the world, lignin valorization not only aligns with the goals of low-carbon and sustainable development but also maximizes the utilization of natural biopolymers. This study employed a novel one-step fractionation method using syringol [*Nature* **2024**, *630*, 381–386] to obtain arylated lignin and high-purity cellulose. The extracted lignin was subsequently epoxidized to synthesize a lignin-based epoxy, which was further combined with commercial filter paper through thermal treatment at various temperatures. By establishing covalent bonds between cellulose and the lignin epoxy, the fiber surface was fully coated by lignin epoxy at microscopic level. Therefore, the tensile strength of this composite (57.8 MPa) was significantly increased compared to untreated filter paper (23.3 MPa). Furthermore, the incorporation of lignin epoxy endows the composite with notable wet strength, expanding its potential applications on packaging materials. This covalently bonded system presents a promising pathway for integrating arylated lignin into bio-based composites, contributing to the efficient utilization of biomass resources and the advancement of sustainable materials.

Keywords: arylated lignin; lignocellulose valorization; bio-based composite; covalent bond

Polymers and Bio-based Materials (PC-O-014)

Flame-retardant coating prepared from prehydrolysis liquors

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Prehydrolysis liquors are produced as a result of hemicellulose removal from biomass during the production of dissolving grade pulp. Currently, prehydrolysis liquors are incinerated to recover energy at low efficiency, hampering pulp production. Presented herein is the preparation and characterization of a biobased polymer synthesized from hemicellulose derived monomers. Quantitative yields of the polymer were achieved by the combination of two monomers, without solvent, in the presence of an acid catalyst at room temperature. It was found that sulfonic acids could be employed to obtain excellent flame-retardant properties. The polymer´s adhesive properties on diverse substrates demonstrates the viability of this material to serve as a versatile flame-retardant coating. Kinetic experiments were used to elucidate the polymerization mechanism and polymer structure. Life-cycle assessment (LCA) was used to evaluate the transformation described herein, in addition to a comparative LCA on this valorization approach, which showed improvements in several impact categories.

Keywords: bio-based materials; hemicellulose; flame-retardant; LCA; kinetics

Polymers and Bio-based Materials (PC-O-015)

Catalytic lignin-arylated fractionation of hemp shives using a biobased nucleophile

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Functionalized lignin-first strategy prioritizes preserving β-O-4 bonds in lignin by averting recondensation to realize holistic valorization of biomass. A hemicellulose derived aromatic nucleophile was used as a capping agent to prevent recondensation to produce arylated-lignin via selective Cα-arylation of lignin. This fractionation approach was studied using model compounds, which showed near quantitative yields. The fractionation of hemp shives was performed in formic acid at varying conditions. At 100°C, 26.3% of arylated lignin was extracted leaving behind 40% residual pulp. The theoretical maximum yield of arylated lignin from hemp shives was calculated to be 29.5%. Unreacted reagents were recovered and reused for further fractionation processes. The pulp could be upscaled to nanocellulose (ligno-nanocellulose) and the arylated lignin can be further functionalized to make biobased polymers and biocomposites, thereby contributing to holistic biomass valorization.

Keywords: arylated lignin; nanocellulose; fractionation; biobased materials; biomass valorization

Polymers and Bio-based Materials (PC-O-016)

Preparation of multifunctional composites for electromagnetic interference (EMI) shielding applications using CuO modified MXene and forestry wastes

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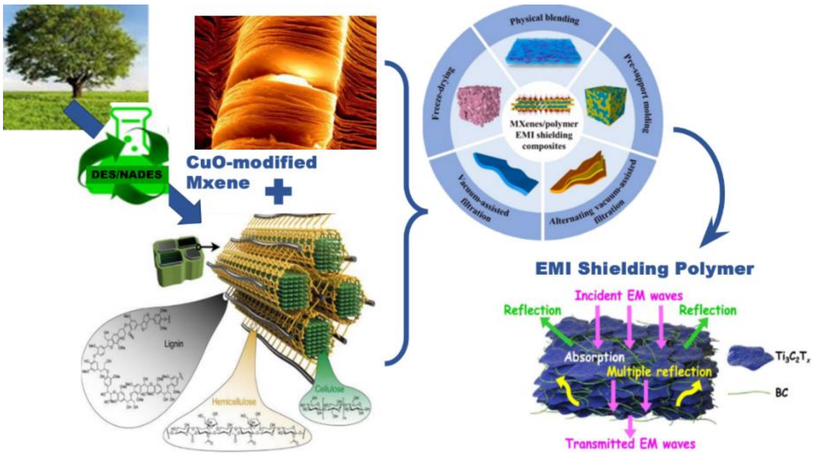
Electronic devices have become an important part of our lives. To meet increasing demand, production of electronic and miniature electronic devices is growing significantly. Unfortunately, this results in higher EMI which impacts our health. Thus, developing effective multi-functional EMI shielding materials are of great importance. This technology requires high conductivity, permeability, permittivity, processability, corrosion resistance while being cost-effective, environmentally friendly materials. There is a need for developing value-added products from sustainable sources. Forestry waste is readily available and thus are among the priority materials to be used as they are listed in all the UN and EU strategy documents.

Cellulose nanofibers (CNFs) have different advantages such as biodegradability, high aspect ratio, processability, and low cost. CNFs can be utilized as a matrix, binder, or derived carbon material for electronic devices. In our study, lignocellulosic components are fractionated from wood waste using non-toxic chemicals of Acidic Deep Eutectic Solvents (ADES) and using hydrothermal (HT) process with less energy and water consumption. The combination of fractioned cellulose fibers and CuO modified MXene will yield a multi-functional composite in different forms (electrospun, aerogel, film, etc.), which will then be used for EMI shielding applications in the whole X-band range (8-12 GHz).

Keywords: electromagnetic interference (EMI) shielding; lightweight; MXene; lignocellulose; nanofibers; electrospinning forestry wastes; MXene; CuO; multifunctional



Polymers and Bio-based Materials (PC-O-019)

Zirconium-based MOF/corncob-derived biopolymer composite for enhancing biogas purification

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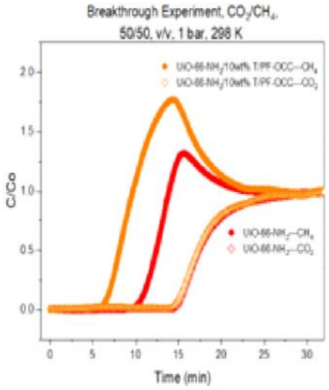
Biogas is a renewable fuel mainly composed of methane (CH_4) and carbon dioxide (CO_2). Biogas upgradation is extremely important; however, it is still challenging to create an efficient approach to removing CO_2 from biomethane. UiO-66-NH_2 is a zirconium-based metal-organic framework (MOF) with polar amine (-NH_2) groups featuring high affinity to CO_2 whereas UiO-66-NH_2 has limited a functional group for CO_2/CH_4 separation. In this study, we investigated functional groups of a corncob-derived biopolymer with UiO-66-NH_2 to form a composite material to improve CO_2/CH_4 separation for biogas upgrading. This biopolymer was produced by converting -OH groups of cellulose into sodium carboxylate and attached to silanol groups. Compared to the pristine UiO-66-NH_2, the composite adsorbent with 10 wt% loading of biopolymer exhibited a 37% increase in CO_2 capacity (2.26 vs. 1.65 mmol/g), and the CO_2/CH_4 (v/v, 50/50) selectivity was improved by 44% (4.78 vs. 3.34) than the parent MOF at 298 K. The efficient CO_2/CH_4 separation for upgrading biogas of the MOF composite was investigated by breakthrough experiments and pressure swing adsorption for 99% CH_4 purity.

Keywords: biogas; UiO-66-NH_2; corncob-derived biopolymer; CO_2/CH_4 separation; PSA process



Polymers and Bio-based Materials (PC-O-020)

Biochemical and structural characterization of lignin from *Trema orientalis* and *Trewia nudiflora* for biorefinery applications

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Trema orientalis and *Trewia nudiflora* exhibit strong anatomical and chemical similarities. Biorefinery research has gained prominence due to its critical role in advancing a circular bioeconomy. In this study, both species were fractionated using formic acid (FA) into pulp, hemicellulose, and lignin. The properties of lignin and its composition vary depending on the raw material and the extraction process used. The lignin extracted from the FA spent liquor was characterized using molecular weight analysis, UV, FTIR, 2D-NMR, and ^{31}P NMR spectroscopy to investigate its structural features and reactivity. The weight average molecular weights (Mw) of the lignins were found to be 10,826 for *T. orientalis* and 8,784 for *T. nudiflora*. The OCH_3/C_9 unit ratios were 1.3 and 1.0, respectively. Both lignins showed nearly identical contents of aliphatic OH (1.23 mmole/g vs. 1.15 mmole/g) and phenolic OH (2.3 mmole/g vs. 2.26 mmole/g). 2D-NMR analysis revealed that both lignins were composed predominantly of S and G units, with S/G ratios of 1.56 for *T. orientalis* and 1.15 for *T. nudiflora*. FA lignin was utilized to partially replace phenol (20%) in phenol-formaldehyde resin synthesis without compromising shear strength. Additionally, the FA lignin, primarily containing pentose sugars, was converted into furfural with yields of 41.39% for *T. orientalis* and 41.72% for *T. nudiflora* at 170 °C using 0.1% H_2SO_4 as a catalyst.

Keywords: hardwood; formic acid treatment; lignin; pentosan; resin; furfural

Polymers and Bio-based Materials (PC-O-024)

Synthesis and characterization of bio-based non-isocyanate polyurethane foam from oil-based polyol with lignin-derivatives for flame-retardant properties

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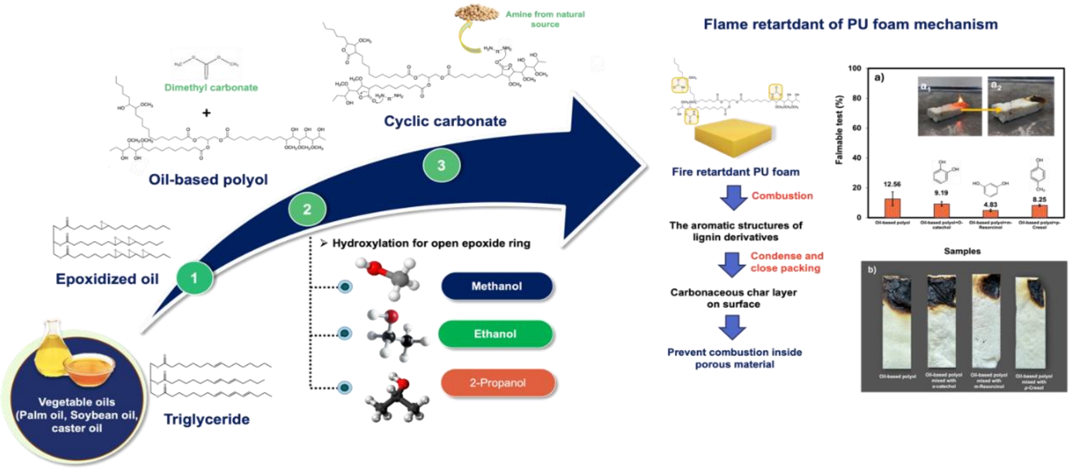
In this work, a green approach for synthesizing non-isocyanate polyurethane (NIPU) foams eliminating the use of hazardous isocyanates is presented. The hard segment of the polymer network was formed via the reaction of cyclic carbonates with bio-based amines derived from the hydrolysis of waste soybean meal, producing urethane linkages through ring-opening aminolysis. The soft segment was derived from oil-based polyols obtained from palm, castor, and soybean oils, which were chemically modified through epoxidation and subsequent hydroxylation using methanol, ethanol, and 2-propanol. Lignin-derived compounds such as o-catechol, m-resorcinol, and p-cresol were incorporated as renewable flame retardants, with m-resorcinol-modified foams exhibiting the best performance, achieving a low mass loss of 4.83% compared to 12.5% for unmodified foams. The incorporation of lignin derivatives also improved the mechanical performance, with modified foams displaying higher energy absorption (2,285–2,625 kJ/m^3) and resilience (>80%), significantly surpassing those of unmodified foams (1,793 kJ/m^3 and ~60% resilience, respectively). DSC analysis revealed semi-crystalline characteristics, with glass transition temperatures ranging from 38.7°C to 48.9°C. The improved flame retardancy was attributed to char formation and radical scavenging mechanisms. The successful synthesis of NIPU foams was confirmed via ^{13}C-NMR spectroscopy. Overall, these results underscore the potential of sustainable NIPU foams enhanced with renewable flame retardants as high-performance materials for thermal insulation applications.

Keywords: non-isocyanate polyurethane; cyclic carbonate; bio-based amines; lignin derivatives; flame-retardant polyurethane



Polymers and Bio-based Materials (PC-O-025)

Areca to eureka: Utilization of areca husk for sustainable packaging and construction in a circular bioeconomy

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Areca husk, the outer cover of the areca nut, is largely discarded and burnt in India, contributing to approximately 6 million tonnes of environmental pollution annually. This study explores sustainable solutions to repurpose this agricultural waste within a circular bioeconomy framework. Primary research indicates that the husk is discarded due to its slow decomposition caused by high lignin content and its potential to spread diseases to areca nut plants. However, its composition—rich in cellulose, lignin, and fiber—makes it a viable raw material for packaging and construction applications.

In this study, areca husk was processed with polyvinyl alcohol as a coupling agent and subjected to high-pressure hydraulic pressing to produce a flexible sheet suitable for packaging. Additionally, a composite particle board was developed by combining areca husk with waste milk sachets in equal proportions. This board, with further refinement, can be used for roofing and wall tiles. The findings demonstrate that areca husk, currently an environmental burden, can be transformed into valuable products, fostering a circular bioeconomy by generating additional income for farmers, creating rural employment, and reducing pollution. This study underscores the potential of agricultural waste valorization in promoting sustainability and economic development.

Keywords: areca husk; circular bioeconomy; sustainable packaging; particle board; waste valorization

Polymers and Bio-based Materials (PC-O-026)

Controllable thermoplasticity and biodegradability of low-substituted cellulose acetate with PLA graft copolymers

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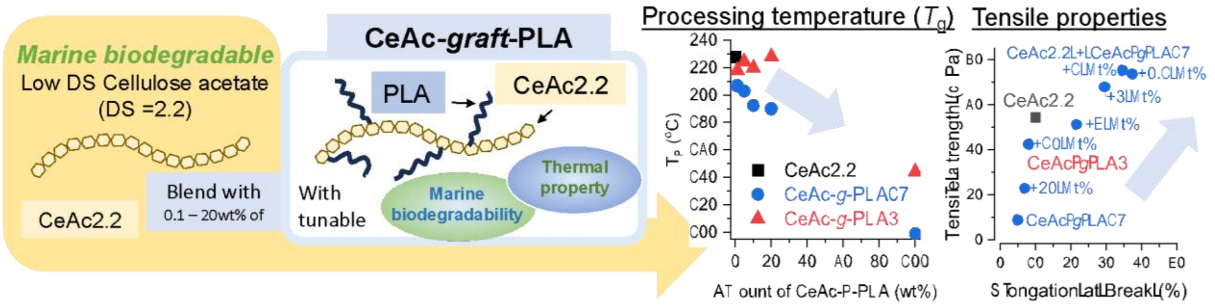
Biodegradable plastics are essential for addressing environmental issues derived by conventional non-biodegradable plastics. This study focuses on enhancing the thermoplasticity and marine biodegradability of cellulose acetate (CeAc) with a low degree of substitution (DS=2.2) via graft copolymerization with poly(L-lactic acid) (PLA) and blending with CeAc. A series of CeAc-*graft*-PLA copolymers were synthesized with various feed ratio. As the degree of polymerization of the PLA side chains (DP_{PLA}) increased, the glass transition temperature (T_g) of CeAc-*graft*-PLA decreased to 60 °C according to DP_{PLA} increase, enabling thermoplastic processing.

Biodegradability was evaluated using a Biological Oxygen Demand (BOD) test in seawater. Longer PLA graft chains led to slower degradation, demonstrating tunable biodegradation behavior. Furthermore, blending CeAc-*graft*-PLA with CeAc2.2 produced miscible blends, allowing for the control of material properties depending on the mixing ratio and DP_{PLA}. Notably, when copolymers with higher DP_{PLA} were blended, even small amounts induced significant changes in CeAc's properties. For instance, blending 30wt% of CeAc-*graft*-PLA17 reduced the T_g to around 180 °C, and the addition of less than 1wt% significantly improved both elongation at break and tensile strength.

This study demonstrates a strategy for designing customizable, marine-biodegradable materials with improved processability and mechanical performance, contributing to the development of sustainable polymer systems.

Keywords: cellulose acetate; poly(L-lactic acid) graft copolymer; control of thermoplasticity; marine biodegradability



Polymers and Bio-based Materials (PC-O-028)

Development and evaluation of enzyme-embedded biodegradable plastics for enhanced environmental degradation

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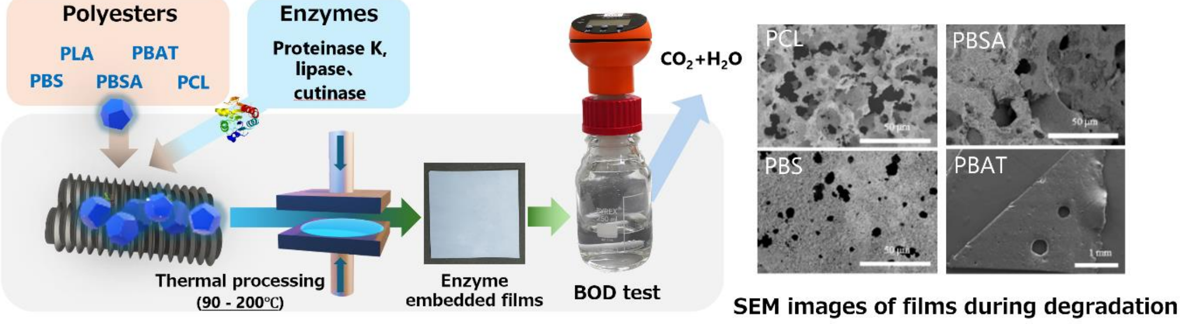
Plastic waste, particularly marine microplastic pollution, is a pressing global issue. Developing high-performance biodegradable plastics offers a potential solution. However, current commercial biodegradable plastics degrade only in specific environments due to the varying presence of microorganisms and their enzymes. For instance, polyesters like PLA, PBAT, and PBS degrade very slowly in marine environments. This research aims to address this limitation by pre-embedding enzymes within plastics, enabling them to decompose in any environment. Upon disposal, water activates the embedded enzymes, initiating degradation. This approach could lead to plastics that remain stable during use but decompose efficiently after disposal.

The study developed poly-L-lactic acid (PLLA) films embedded with Proteinase K, an enzyme that degrades polylactic acid. Films created via the casting method showed 80% weight loss in four days, while the thermal kneading method resulted in slower degradation. To enhance performance, ProK was immobilized on polyacrylamide gel beads, increasing decomposition rates by 2.5 times. Additionally, embedding lipase and cutinase into biodegradable polyesters via thermal kneading demonstrated rapid degradation in water, with seawater tests confirming biodegradability comparable to cellulose. Finally, modifying enzymes with polyethylene glycols (PEG) improved thermal stability and activity, enabling significant degradation of enzyme-embedded poly-D-lactide (PDLA) films in both buffer and seawater.

Keywords: biodegradable polymer; polyester; enzyme; thermal processing



Physical and Theoretical Chemistry (PT-O-003)

Lantern organic frameworks:
A new 3D material concept from computer-aided design

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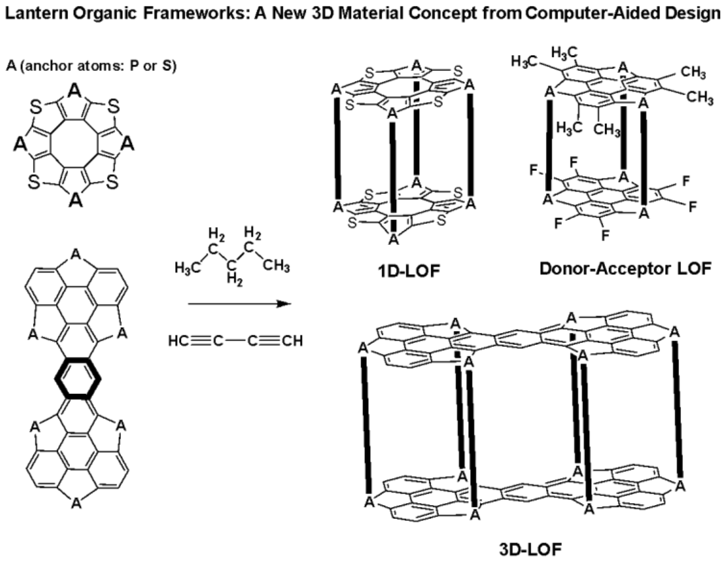
Lantern Organic Frameworks (LOFs) have developed from a computational concept into a promising class of tunable materials. Initially, 1D-LOFs were designed using Density Functional Theory (B3LYP-D3/6-31+G(d)), with circulene bases linked by sp^3- and sp-carbon bridges anchored by phosphorus and silicon. These stacked structures maintained stable electronic properties, making them suitable for porous materials and host–guest chemistry. Expanding into 3D-LOF, we introduced trisilasumanene and porphyrin cores connected by benzene linkers and silicon-anchored bridges. This shift allowed for tunable porosity while maintaining electronic properties driven by the core unit. The latest advancement functionalizes LOFs into donor–acceptor mixed stacking cocrystals, where covalent bonding enhances stability over non-covalent systems. By incorporating electron-donating and withdrawing groups, we achieved tunable bandgaps (1.50–3.50 eV) and improved conductivity via Yoshizawa's model. This development establishes LOFs as a new frontier in material design, balancing structural precision with functional versatility for applications in electronics, catalysis, and energy storage.

Keywords: lantern organic framework; circulenes; trisilasumanene; porphyrin; covalently bonded mixed stacking



Thailand-Japan Bilateral Symposium: Advancing Synchrotron Science through Experimental and Computational Chemistry Synergy (S1-O-001)

In-situ QXAFS study of CO_2 adsorption behavior on Nb and Ta heteropolyoxometalate

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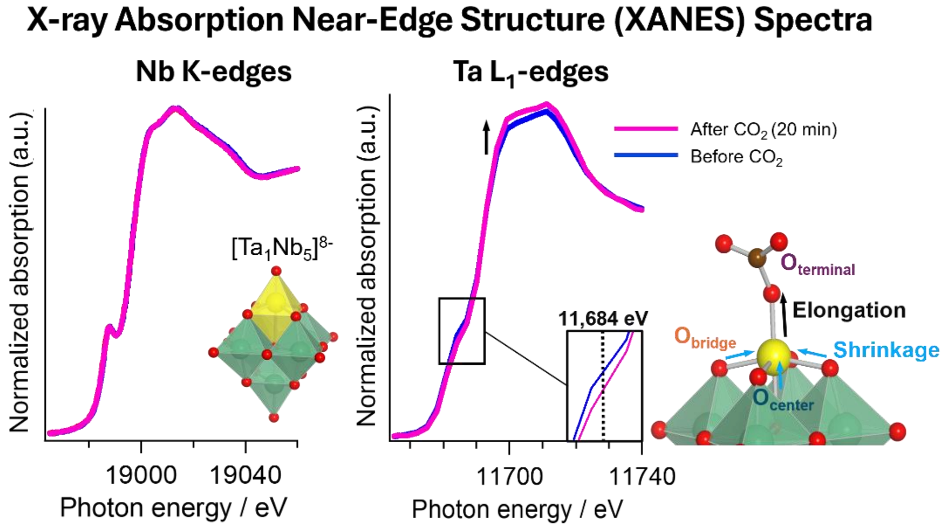
Polyoxometalates (POMs) composed of Ta and Nb possess base properties that facilitate catalytic activity for Knoevenagel condensation and CO_2 fixation reactions [*J. Phys. Chem. C.* 2018, 122, 29398–29404]. Recently, we have reported Tetrabutylammonium (TBA) salts of Ta–Nb heteropolyoxometalate, $TBA_mH_n(Ta_xNb_{6-x}O_{19})^{(8-m-n)-}$ (referred as TBA-Ta_xNb_{6-x}), to promote CO_2 fixation reaction to styrene [*Catalysts*, 2023, 13, 432–442]. Especially, TBA-Ta_1Nb_5 promoted CO_2 fixation to styrene oxide to form styrene carbonate (SC) with high selectivity while other compositions showed low SC selectivity. Thus, the behavior of single Ta site in TBA-Ta_1Nb_5 is of interest. Accordingly, this work focuses on monitoring the CO_2 adsorption behavior by using the time-resolved quick X-ray absorption fine structure (QXAFS). TBA-Ta_xNb_{6-x} fabricated by microwave-assisted hydrothermal synthesis was characterized by ESI-MS, FT-IR, and elemental analysis. The *in-situ* QXAFS showed the structural changes in 20 min for ca. 1 equimolar CO_2 adsorption on a unit of TBA-Ta_1Nb_5. The changes in XANES spectra were observed in Ta L_1-edge, while no significant changes in the Nb K-edge. These results and DFT calculations suggest that the TaO_6 unit in TBA-Ta_1Nb_5 acted as the main CO_2 adsorption site accompanied with the structural change of TaO_6 unit.

Keywords: polyoxometalates; base catalysts; CO_2 fixation reaction; CO_2 adsorption; QXAFS



Catalytic Systems for Contemporary Challenges (S2-O-003)

Novel nickel phosphite/NHC precatalysts for cross coupling reactions under mild conditions

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The synthesis and catalytic properties of Ni(II) complexes, with the general formula Ni(NHC)[P(OR)$_3$](Ar)Cl will be discussed. These complexes are air-stable and extremely effective precatalysts for both the Suzuki-Miyaura and C-N cross-coupling reactions. The reaction protocols described allow for the cross-coupling of aryl chlorides employing low catalytic loading, to deliver a large variety of functionalized biaryl and amine compounds. Overall, these reaction protocols operate at room or mild temperatures and can be applied to a variety of electronically and sterically differentiated coupling partners. Fundamental insights into the mechanism of this reaction, including the proposed formation of the catalytically active Ni(NHC)[P(O*i*-Pr)$_3$] complex and resting state species will also be discoursed.

Keywords: nickel; catalysis; cross-coupling; room temperature; mechanism

Catalytic Systems for Contemporary Challenges (S2-O-007)

Ruthenium catalyzed additive-free N-formylation of amines with CO_2 and H_2: Exploring carbon neutral hydrogen cycle

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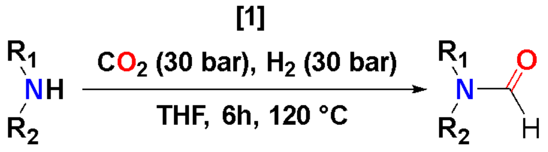
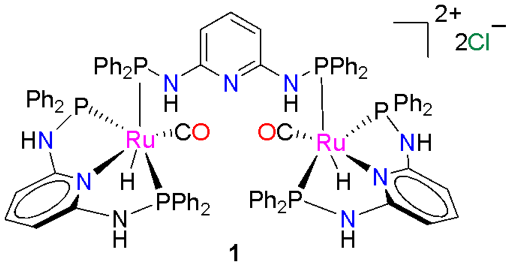
Production of bulk and value-added chemicals using abundant and inexpensive CO_2 as C1 building block has the potential to become an essential part of the sustainable chemical industry. [*Nat. Commun.* **2015**, *6*, 5933] However, the thermodynamic stability and kinetic inertness of CO_2 pose a significant challenge for such a methodological development. The design of catalytic systems to overcome these issues is thus of principal research interest. CO_2 can be utilized in N-formylation of amines, where it acts as carbonyl source in N-formylation of amines. Formamides are considered as important intermediate in synthesis of value added chemicals, namely, pharmaceutical materials, N-heterocycle, oxazolidinones and cancer agents. [*Angew. Chem. Int. Ed.* **2012**, *51*, 9226–9237] Herein, we report a ruthenium-pincer-type complex as a highly efficient catalyst towards N-formylation of amines with CO_2 and H_2. [*ChemCatChem* **2024**, *16*, e202401202] A variety of amines are converted to their corresponding formamides with excellent reactivity and selectivity. A maximum TON of 980,000 was attained under a single-batch condition, indicating the potential application of these processes in industrial settings. In addition, this methodology was examined to establish a carbon neutral hydrogen storage cycle by capitalizing on the reversible transformation of formamides.

Keywords: CO_2 utilization; N-formylation; catalysis; pincer complex



- ♦ **No External Additive**
- ♦ **Mild Reaction Condition**
- ♦ **Wide Substrate Scope**
- ♦ **Water as only byproduct**
- ♦ **Atom Economically Favoured**
- ♦ **High TON: 980000**



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Catalytic Systems for Contemporary Challenges (S2-O-008)

Wireless flux reactors for asymmetric electrosynthesis using green chiral media

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Asymmetric synthesis of enantiopure compounds is a field of high importance, especially in the pharmaceutical industry. In this work, we present a wireless flux reactor for asymmetric electrosynthesis, exploiting the synergy between bipolar electrochemistry and chiral ionic liquids. Our device consists of a polypyrrole (Ppy) tube that acts as a wireless miniaturized electropump, [*Chem* **2024**, *10*, 1–15] driven by an external electric field, to ensure efficient mass transport of the prochiral substrate. Inside the tube, the prochiral precursor is dissolved in droplets of chiral ionic liquids, providing a chiral environment for enantioselective reactions. [*submitted*] We have demonstrated the effectiveness of this approach exploiting the enantioselective reduction of acetophenone to 1-phenylethanol as a model reaction. By optimizing the electric field and reaction time, we were able to obtain 1-phenylethanol with high enantiomeric purity and high conversion efficiency. This wireless and sustainable method offers an environmentally friendly alternative for the production of enantiopure compounds, with promising applications in the pharmaceutical, chemical, and materials science fields.

Keywords: bipolar electrochemistry; asymmetric electrosynthesis; flux reactors; chiral ionic liquids; electromechanical pumping

Catalytic Systems for Contemporary Challenges (S2-O-009)

Direct catalytic conversion of xylose into furfuryl alcohol over bifunctional acid-nickel porous carbon catalysts

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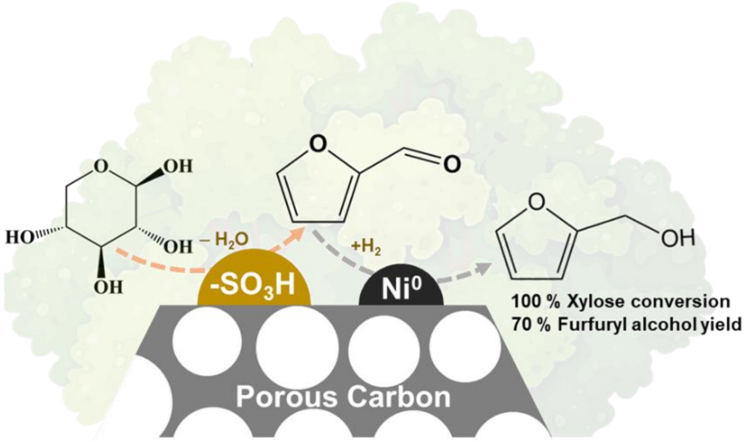
In recent years, a significant amount of focus has been placed on catalytically dehydrating xylose to produce furfural (FF), followed by selective hydrogenation of FF to produce furfuryl alcohol (FA), a key intermediate for producing a variety of high-value chemicals. Conventional heterogeneous catalysts typically require a two-step process for this conversion and often involve complex preparation methods utilizing costly or hazardous chemicals. In this study, efficient bifunctional acid-Ni porous carbon catalysts (SO_3H@NiMC) were synthesized through a straightforward and efficient process and applied for the direct conversion of xylose to FA. The catalysts exhibited excellent physicochemical properties, achieving complete xylose conversion (100%) and high FA selectivity (70%) in a one-pot process under optimized conditions (170 °C, 1 h). Notably, the predominant presence of metallic Ni eliminated the need for an additional Ni reduction step, which is typically required for conventional metal-based catalysts. These findings further underscore the potential of SO3H@NiMC as an advanced and sustainable catalyst for the scalable production of FA. Its high catalytic efficiency, combined with process simplification and reduced environmental impact, makes it a promising candidate for industrial applications, thus offering both economic and environmental advantages.

Keywords: direct conversion; furfuryl alcohol; bifunctional catalyst; mesoporous carbon; xylose



Catalytic Systems for Contemporary Challenges (S2-O-013)

Selective imine synthesis by supported Ag nanoparticle catalyst modified with basic polyoxometalate

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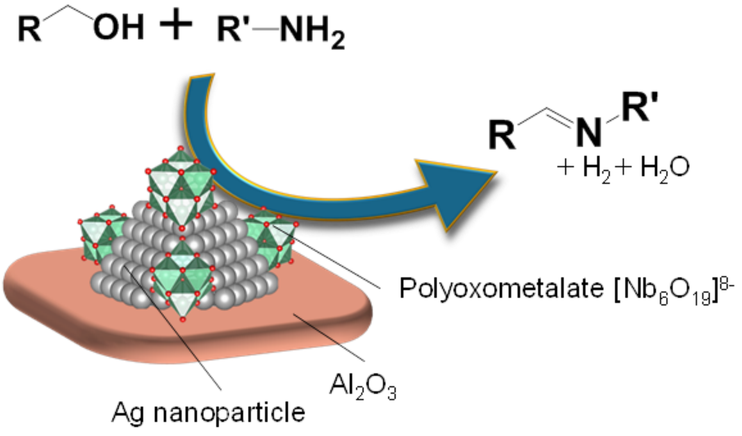
The composite materials of supported metal nanoparticle (NP) catalysts, of which the surface was modified with polyoxometalates (POMs), have been developed by a simple adsorption method, exhibiting the bifunctionality of redox ability of metal NPs with Lewis basicity of POMs. [*Chem. Commun.* **2022**, *58*, 9018–9021; *Catal. Soc. Technol.* **2025**, *15*, 2466–2472] In this study, we developed Al_2O_3-supported Ag nanoparticles (Ag NPs) with a surface modification with POM (POM-Ag/Al_2O_3), which has multifunctional properties: Lewis basicity of polyoxoniobate $[Nb_6O_{19}]^{8-}$, oxidative dehydrogenation activity of Ag NPs, and Lewis acidity of Al_2O_3 support. POM-Ag/Al_2O_3, which was synthesized by selective adsorption of basic $[Nb_6O_{19}]^{8-}$ on the Ag NPs surface, selectively produced imines by acceptorless dehydrogenative coupling of various alcohol and amines. Acceptorless dehydrogenation of alcohol accompanied with H_2 production took place at the interface between the Ag NPs surface and $[Nb_6O_{19}]^{8-}$, followed by the dehydrative condensation of amines and aldehydes on the Lewis acid sites of Al_2O_3. This study proved the selective imine synthesis with H_2 production over Ag-based catalysts whose surface was designed by basic POMs.

Keywords: multi-functional catalyst: supported Ag nanoparticle; polyoxometalate; acceptorless dehydrogenative coupling; imine synthesis



Selective imine synthesis via acceptorless dehydrogenative coupling by tri-functional POM-Ag/Al_2O_3

Catalytic Systems for Contemporary Challenges (S2-O-014)

Tailoring metal-organic frameworks for enhanced ammonia production through non-thermal plasma catalysis

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This work investigates the non-thermal plasma (NTP)-catalysed synthesis of ammonia (NH_3) as an energy-efficient alternative to conventional, fossil-fuel-intensive production methods using metal-organic frameworks (MOFs) as highly tunable catalytic platforms. The thermally and chemically stable UiO-66-based MOFs were systematically modified via two distinct strategies: transition-metal doping (Ni, Co, Cu, and Ru) and linker functionalisation (-H, -NH_3, and -OH) to optimise their catalytic performance. Comprehensive solid-state characterisation, including PXRD, XPS, XAS, IR spectroscopy, N_2 sorption analysis, and TPD measurements, revealed strong interactions between metal ions and MOF frameworks, generating open metal sites (OMS) that are suitable for small molecule adsorption and activation. The metal-doped MOFs exhibited exceptional catalytic activity and stability, with Ni@UiO-66-NH_2 achieving energy efficiencies up to 1.3 gNH_3/kWh, outperforming many conventional catalysts. Importantly, the catalytic trends in NTP-driven reactions differ from thermal catalysis, possibly due to distinct metal-binding interactions with key intermediates under plasma conditions. These insights underscore the promise of MOFs as adaptable catalysts for sustainable NH_3 synthesis, with future research opportunities in mechanistic elucidation and in situ analysis. This study illustrates the feasibility of MOF-based catalysts in promoting green chemistry and enhancing energy-efficient NH_3 synthesis.

Keywords: metal-organic frameworks; ammonia production; non-thermal plasma catalysis; transition-metal doping; linker functionalisation

Metal-acetylide frameworks: Synthesis, characterization, and optical and catalytic properties

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The novel metal-acetylide frameworks (MAFs) has been designed and synthesized with homo- or hetero-metallic skeleton via the facile bottom-up method, which integrates the advantages of both metal centers and graphdiyne frameworks. The propensity of d_{10} Hg(II)-, d_8 Ni(II)-, Pd(II)- and Pt(II)-$(PR_3)_2$ (R = alkyl chain) units to form a moiety with alkynyl units makes them attractive building blocks for 2D organometallic functional materials. The ligand structures and electronic properties can be easily adjusted in terms of the spacer length between the ethynyl unit and central core, central chromophore as well as the number of coordination sites. Therefore, the 2D nanosheets with different topological structures, pore sizes, surface areas and advanced functionalities can be prepared by using different monomers with diverse electronic, optical and catalytic properties. The relationship between the performance of MAFs and their well-defined nanostructures will be elucidated, with a major focus on studying the effects of transition metals and ligands in activating their optical and catalytic properties. The properties and catalytic performance can be fine-tuned through chemical modification of the chromophores. The proposed work can produce a new class of 2D carbon-rich materials and provide a design concept for developing efficient nonlinear optical materials and photo-/electro-catalysts. [*Angew. Chem. Int. Ed.* **2021**, *60*, 11326; *Nano Today* **2022**, *43*, 101428; *J. Am. Chem. Soc.* **2022**, *144*, 15143; *Angew. Chem. Int. Ed.* **2025**, 64, 202418269; *Nano Energy* **2025**, *136*, 110685]

Keywords: metal-acetylide frameworks; 2D nanomaterials; topological structure; nonlinear optic; catalyst

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-O-001)

Eco-friendly fabrication of copper oxide nanoparticles via *Azadirachta indica* and *Curcuma longa* extracts: Unlocking potent antibacterial potential

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The rapid rise of antimicrobial resistance is a pressing global health challenge, necessitating sustainable alternatives to conventional medicines. Green nanoparticle synthesis using medicinal plants like *Curcuma longa* (turmeric) and *Azadirachta indica* (neem) offers an eco-friendly solution, leveraging their inherent antimicrobial properties. This study presents the green synthesis of copper oxide nanoparticles (CuO NPs) using biomolecule-rich extracts from these plants, acting as natural cappers and stabilizers. Ethanol and n-hexane were employed for efficient bioactive compound extraction, enhancing nanoparticle activity.

Characterization techniques, including UV/Vis spectroscopy, EDX, FE-SEM, XRD, and FTIR, confirmed particle sizes between 50–150 nm, with 1D nanorods and 0D nanoclusters as predominant morphologies. Antimicrobial efficacy was tested against *Bacillus subtilis* and *Escherichia coli* using agar well diffusion. Ethanol-based formulations exhibited larger inhibition zones compared to n-hexane, demonstrating significant activity even at low concentrations (50–150 mg/mL).

This scalable and green approach highlights the potential of plant-mediated CuO NPs to combat drug-resistant infections, integrating green chemistry and nanotechnology for sustainable antimicrobial development. This work provides a promising pathway for addressing antimicrobial resistance with implications in healthcare, environmental sustainability, and materials science.

Keywords: Green synthesis, copper oxide nanoparticles, antimicrobial resistance, *Curcuma longa*, *Azadirachta indica*

Evaluation of the antioxidant and antibacterial activities of the crude extract of *Rhinacanthus nasutus*

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In this study, the antioxidant activity of *Rhinacanthus nasutus* crude extract obtained using methanol was evaluated using the DPPH assay, along with its antibacterial activity. The methanol crude extract exhibited antioxidant activity with a DPPH scavenging value of 27.81 ± 2.17%. Antibacterial activity against *Staphylococcus aureus* (*S. aureus*) ATCC 25923 was assessed using the agar disc diffusion method at concentrations of 500 and 1000 mg/mL. The results showed that the methanol crude extract of *Rhinacanthus nasutus* was most active against *S. aureus* ATCC 25923, with inhibition zones of 8.06 ± 0.17 mm and 8.00 ± 0.33 mm at 500 and 1000 mg/mL, respectively. These findings indicate that the methanol crude extract of *Rhinacanthus nasutus* possesses notable antioxidant and antibacterial activities. Therefore, it is a promising candidate for further characterization to identify its chemical constituents and to evaluate its bioactivity against other bacterial strains.

Keywords: *Rhinacanthus nasutus*; antioxidant activity; crude extraction; antibacterial activity

Green Chemistry; Paving the Way to a Sustainable Future (S8-O-001)

Environmentally friendly electrodeposition of conducting polymers using supercritical carbon dioxide-with-water emulsified electrolytes

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Conducting polymers, such as polypyrrole (PPy), and poly(3,4-ethylenedioxythiophene) (PEDOT), are attractive materials due to their unique organic semiconductor characteristics. However, the preparation of them often requires toxic and harmful organic solvents and oxidants. To overcome this problem, the electrodeposition performed in supercritical carbon dioxide ($scCO_2$)-with-water ($scCO_2/H_2O$) emulsified electrolyte is a green alternative because electropolymerization requires no oxidant, and both $scCO_2$ and H_2O are green solvents. Given these motivations, this research reports the electrodeposition of PPy and PEDOT using the $scCO_2/H_2O$ emulsified electrolyte, and investigation of their morphologies and optoelectronic properties. After the electrodeposition of PPy (PEDOT) using a Pt plate as a working electrode, the desired polymer film was deposited onto the substrate. PPy showed a black film, whereas PEDOT had a blue film. SEM observation showed that PPy had cauliflower-like structured and PEDOT had a thin film with small particles. Their morphologies could be controlled by changing the electrolyte components and the properties of $scCO_2/H_2O$ emulsified electrolyte. The effects of them and substrate materials on the various properties of PPy and PEDOT are also given in the presentation. In conclusion, PPy and PEDOT were successfully electrodeposited in $scCO_2/H_2O$ emulsified electrolyte, which provides a greener approach for preparing conducting polymers.

Keywords: conducting polymer; polypyrrole; poly(3,4-ethylenedioxythiophene); electropolymerization; supercritical carbon dioxide-with-water ($scCO_2/H_2O$) emulsified electrolyte; green processes

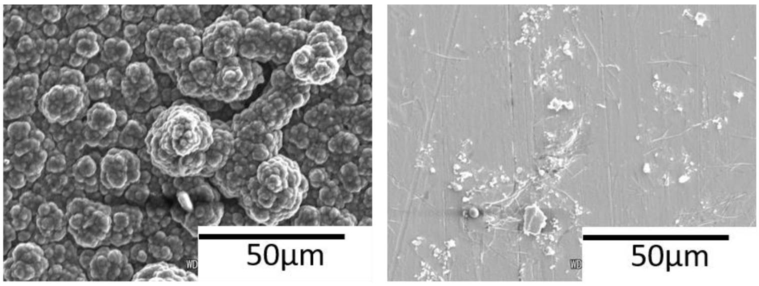

Figure: SEM images of PPy (left) and PEDOT (right)

Green Chemistry; Paving the Way to a Sustainable Future (S8-O-006)

Self-powered water purification using a hybrid piezoelectric-photocatalytic system

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One of the biggest challenges facing the world today is water scarcity and pollution. These issues most certainly call for more cost-effective and energy- wise purification facilities. This work report's on a self-powered water purification system that features the integration of piezoelectric nanogenerators with photocatalytic nanomaterials for effective pollutant degradation and disinfection. The system captures flowing water mechanical energy using a ZnO-based piezoelectric nanogenerator which then supplies electric power to a TiO2-graphene oxide (GO) photocatalyst working under ambient light. By combining these two methods, the system is able to utilize the ROS produced to a greater extent, resulting in higher rates of organic contaminant removal using microbial disinfection, without any needed power supply. Laboratory tests show that within 30 minutes, 90% of contaminants are removed which makes this solution cost-effective and economically scalable to implementing decentralized water treatment facilities. This work helps the application of research done in green chemistry, clean energy and sustainable purification of water.

Keywords: self-powered; water purification; piezoelectric; photocatalysis; sustainable chemistry

Effective hydrothermal carbonization and sulfonation of water hyacinth husk to prepare a carbonaceous catalyst for the dehydration of xylose to furfural

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Furfural is a key platform chemical with diverse industrial applications. In this study, a carbon-based catalyst (WC-SO_3H) was synthesized from water hyacinth husk using hydrothermal carbonization and sulfonation. WC-SO_3H was utilized to convert xylose into furfural in dimethyl sulfoxide. The structural and compositional analyses of the catalyst were investigated by various techniques including Fourier transform infrared spectroscopy, X-ray diffraction, energy-dispersive X-ray spectroscopy, scanning electron microscopy, and elemental mapping. Numerous factors, namely solvent type, substrate concentration, catalyst loading, reaction temperature, and reaction time were proved to influence furfural yield. The highest furfural yield of 68.1% was achieved at 140 °C after 14 h. Additionally, the catalyst's recyclability and the scalability of the process were also assessed.

Keywords: solid acid; carbonaceous material; furfural; xylose

Photocatalytic non-oxidative coupling of methane over Ag-doped ZnO/TiO_2-SiO_2 composite catalysts

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The photocatalytic non-oxidative coupling of methane represents a promising approach for converting methane into valuable higher hydrocarbons under mild conditions. This study investigates the effect of Si to Ti ratio on the performance of Ag-doped ZnO/TiO_2-SiO_2 composite photocatalysts while maintaining fixed contents of Ag and ZnO. The photocatalysts were synthesized using a hydrothermal method and characterized by X-ray diffraction (XRD), UV-vis diffuse reflectance spectroscopy, N_2 physisorption, and scanning electron microscopy (SEM). The photocatalytic activity was evaluated for non-oxidative methane coupling under xenon light irradiation. Density functional theory (DFT) calculations were performed to understand the electronic properties and methane adsorption mechanisms on the catalyst surface at different Si to Ti ratios. The correlation between experimental observations and theoretical calculations provides insights into the role of Si to Ti ratio in determining catalyst performance. This study aims to establish structure-property relationships and optimize the composition of composite photocatalysts for efficient methane conversion.

Keywords: photocatalysis; methane; Ag doping; silica-titania composites; DFT

Green Chemistry; Paving the Way to a Sustainable Future (S8-O-010)

Kinetic model analysis and response surface methodology optimization in citronella leaves extraction using microwave hydro-distillation and solvent-free microwave extraction

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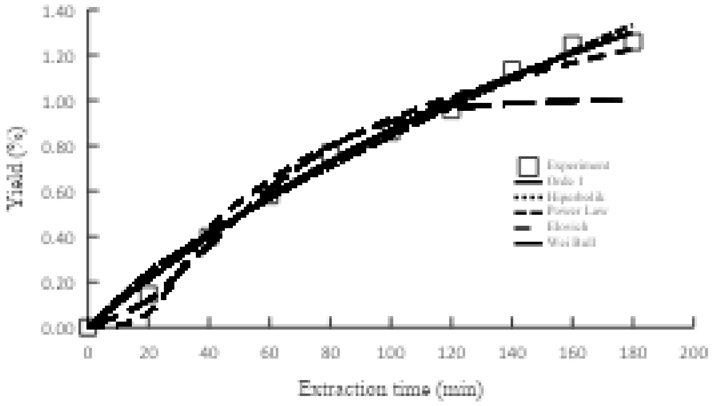
Microwave-assisted extraction methods have shown significant advancements in essential oil extraction processes. Among these, microwave hydro-distillation (MHD) and solvent-free microwave extraction (SFME) have been recognized for their ability to produce high-quality essential oils. This study aims to analyze the kinetic model and optimize the extraction process using response surface methodology (RSM) for both methods. The variables include feed-to-solvent (F/S) ratios of 0.1, 0.15, and 0.2 g/ml, microwave powers were 150, 300 and 450 watt and extraction time for 180 minutes with 20 minutes interval. The result suggest that the hyperbolic model was slightly better at representing the experimental data of MHD. Based on the RSM optimization, the highest results using the MHD method were the F/S ratio of 0.5 cm, microwave power at 450 W and extraction time of 180 min result yield of 2.091%.

Keywords: citronella; microwave; kinetic model; response surface methodology; central composite design



Green Chemistry; Paving the Way to a Sustainable Future (S8-O-020)

Data-driven strategies for accelerated MOFs design and synthesis

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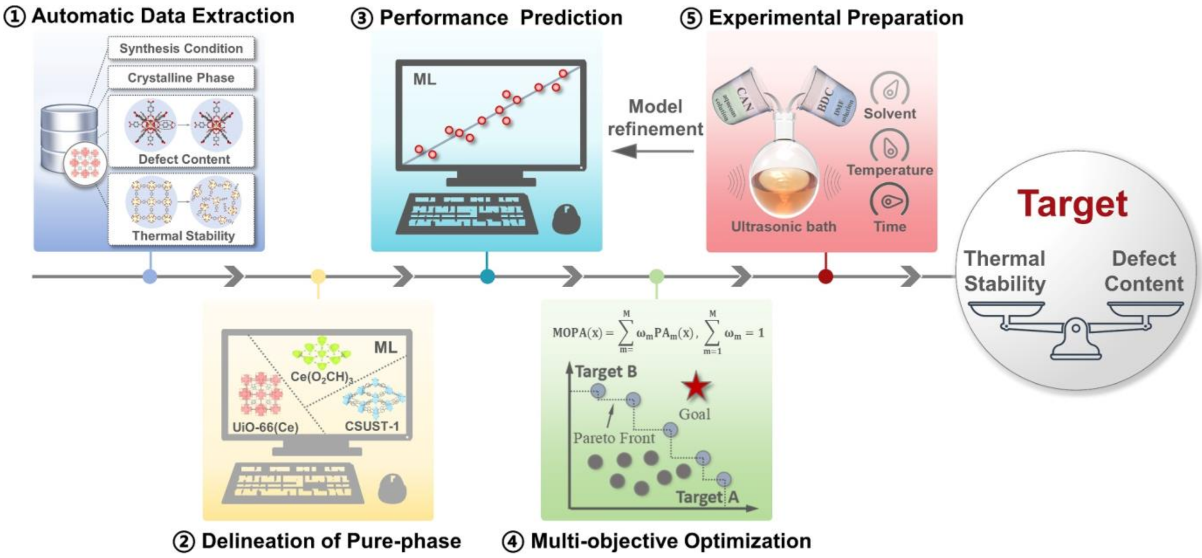
Metal-organic frameworks (MOFs) is a new class of nanoporous material that is widely used in catalytic field due to their large specific surface area, high porosity and tunable pore size. Its excellent chemical tunability provides a wide material space, in which tens of thousands of MOFs have been synthesized. However, it is impossible to explore such a vast chemical space through trial-and-error methods, making it difficult to achieve custom design of high-performance MOFs for specific applications. By employing three descriptors-RACs, SOAP, and the Henry constant, we trained machine learning (ML) models. These models attained an outstanding Macro - AUC score of 0.82 when predicting the water stability of MOFs, all the while showcasing robust generalization capabilities and high reliability. Through data techniques (correlation analysis, genetic algorithm, crystal graph convolutional neural network), exploring the correlation between catalytic activity with metal active site composition and local chemical environment. By using the multi-objective optimization approach with a small number of iterations of experiments, providing a methodology for the co-optimization of defects and stability of Ce-MOF, guiding the optimization to improve the existing Pareto frontiers and enabling the optimal design of MOF catalyst with the best overall performance.

Keywords: metal-organic frameworks; machine learning; water stability; catalyst



TU-Frontier Lab-JEOL joint session Contaminants of Emerging Concern: PFAS & Microplastics (SB-O-001)

Covalent organic frameworks for the detection and removal of perfluorooctanoic acid from water

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Per- and polyfluoroalkyl substances (PFAS) contamination in water poses a severe environmental and public health challenge due to their persistence and toxicity. In this study, we present a cationic covalent organic framework (COF), TG-PD COF, designed for the efficient detection and removal of perfluorooctanoic acid (PFOA), a widely used and highly toxic PFAS compound. Synthesized via a sonochemical method, TG-PD COF exhibits high porosity, well-distributed cationic adsorption sites, and a dual-mode interaction mechanism combining hydrophobic and electrostatic interactions. The material demonstrates remarkable sensitivity and selectivity for PFOA detection, with a fluorescence turn-on response and a detection limit as low as 1.8 µg/L. In adsorption studies, TG-PD COF achieves rapid and high-capacity PFOA removal, with an adsorption capacity exceeding 2600 mg/g in batch experiments and complete removal at environmentally relevant concentrations in continuous flow systems. The adsorption mechanism, elucidated through experimental and computational studies, reveals cooperative adsorption behavior driven by molecular aggregation and strong ionic interactions. These findings highlight the potential of TG-PD COF as a promising material for PFAS remediation, offering a viable approach for addressing the widespread contamination of these persistent pollutants. A first story from this work was recently published in *Nature Communications* (https://doi.org/10.1038/s41467-024-53945-4).

Keywords: PFAS; PFOA; covalent organic framework; adsorption; water treatment; fluorescence sensing

TU-Frontier Lab-JEOL joint session Contaminants of Emerging Concern: PFAS & Microplastics (SB-O-002)

Detection of PFAS by diblock copolymer PS-b-P4VP in complex emulsions at ppb levels

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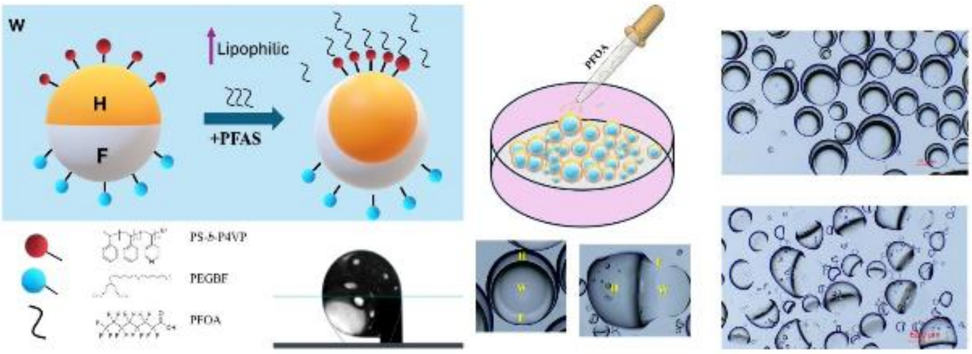
This study explores the use of polystyrene-block-poly(4-vinylpyridine) (PS-*b*-P4VP) diblock copolymers as effective stabilizers for complex triple emulsions, particularly for the detection of per- and polyfluoroalkyl substances (PFAS) in aqueous environments. The amphiphilic nature of PS-*b*-P4VP enables it to significantly manipulate interfacial tension and stabilize liquid-liquid interfaces, facilitating the encapsulation of water layers within hydrocarbon and fluorocarbon phases. We synthesized PS-*b*-P4VP with varying monomer ratios and employed a vortex method to prepare complex emulsions, observing notable morphological transformations upon the introduction of PFAS. The interaction between the P4VP segment of the copolymer and PFOA leads to alterations in droplet morphology, which can be quantitatively assessed through MWFC (multi-well flow chips) changes in morphological properties at low detection levels. Our results demonstrate that these emulsions can serve as responsive platforms for PFOA detection, showcasing their potential application in environmental monitoring. This work highlights the versatility of BCPs in emulsion stabilization and their critical role in developing advanced sensing mechanisms for hazardous substances.

Keywords: emulsions; PFAS; PDMS microfluidics; detection



Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-O-001)

Enhancing ionic conductivity in $LiFePO_4$ composite cathodes for solid-state batteries through dispersed LLZTO

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Enhancing the ionic conductivity of $LiFePO_4$ cathodes in solid-state lithium-ion batteries requires the effective integration of $Li_{6.75}La_3Zr_{1.75}Ta_{0.25}O_{12}$ (LLZTO), a chemically stable and ion-conductive material. This study demonstrates that the distribution of LLZTO particles plays a crucial role in determining conductivity improvements. A solid-state battery with a pristine $LiFePO_4$ cathode exhibited an initial capacity of 146 mAh g^{-1} at 0.2C but retained only 26% capacity after 100 cycles. When LLZTO was incorporated in an agglomerated state, the initial capacity remained similar, but retention dropped below 20%. However, a well-dispersed LLZTO incorporation led to a significant improvement, raising the initial capacity to 160 mAh g^{-1} and achieving a retention rate above 95%. Finite element analysis simulations revealed that agglomerated LLZTO disrupts Li^+ transport, causing localized deficiencies and non-uniform conductivity, ultimately impairing battery performance. These findings highlight the importance of LLZTO dispersion in optimizing the electrochemical properties of $LiFePO_4$ cathodes.

Keywords: Li-ion battery; ionic conductivity; composite $LiFePO_4$ electrode; LLZTO; FEA simulation

Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-O-002)

DNA aptamer (LepDapt) against Lipl32 as a potential diagnostic agent for detection of Leptospira

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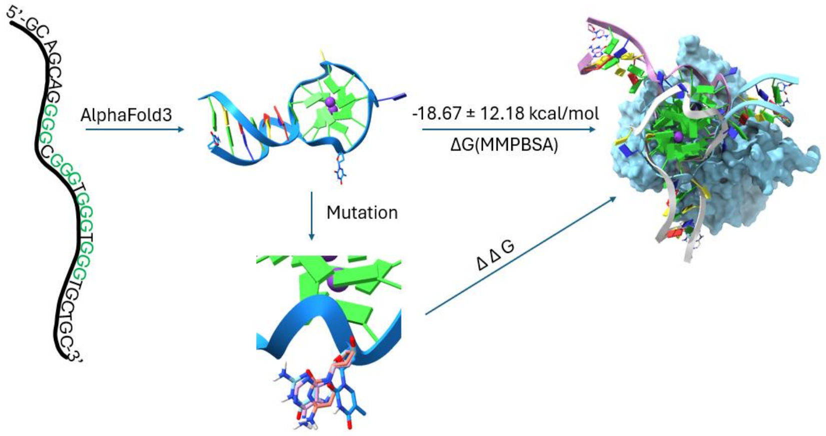
Leptospirosis is caused by pathogenic Leptospira bacteria. For rapid and direct detection of the infection, DNA aptamers (LepDapt) were developed to target LipL32, the most abundant outer membrane protein in Leptospira species, using Systemic Evolution of Ligands via Exponential Enrichment (SELEX). Among the identified candidates, LepDapt-5a exhibited the strongest binding affinity, with dissociation constants (K_d) of 33.97 ± 5.30 nM and 46.35 ± 9.09 nM. Despite these promising binding affinities, the structure details and mechanism of these aptamers with LipL32 remain unclear. To address this, we employed AlphaFold3 to predict the 3D structure of the DNA aptamers and used the HADDOCK2.4 webserver to model their binding interactions with LipL32. Molecular Dynamics (MD) simulations were performed for all complexes using AMBER ff14SB force field for Protein and AMBER OL15 for DNA. Analysis confirmed that LepDapt-5, LepDapt-5a and LepDapt-5b adopt G-Quadruplex structure. The free-energy binding for LepDapt-5a with LipL32, calculated using Molecular mechanics Poisson-Boltzmann surface area (MMPBSA) method, was estimated to be -18.67 ± 12.18 kCal/mol, which agrees with the experimental dissociation constant.

Keywords: DNA aptamer; leptospirosis; MD simulations; alchemical MD



Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-O-004)

Enhanced electrochemical performance of $NiTiO_3$ via $NaBH_4$ reduction for supercapacitor applications

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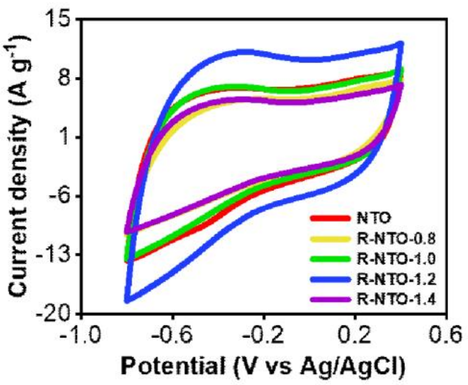
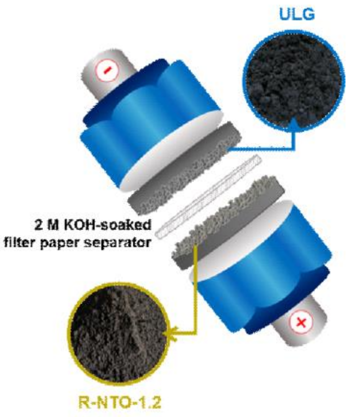
The increasing demand for efficient energy storage necessitates the development of high-performance electrode materials. Nickel titanate ($NiTiO_3$) shows potential for supercapacitor applications; however, its low conductivity and structural instability limit its performance. In this study, oxygen vacancy-enriched $NiTiO_3$ (R-NTO) was synthesized via a simple solid-state, solvent-free grinding process using $NaBH_4$ as a reducing agent. Structural and electrochemical characterizations, including X-ray diffraction (XRD), Raman spectroscopy, infrared spectroscopy (IR), cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS), confirmed the successful synthesis. Among the samples, R-NTO-1.2 exhibited a high specific capacitance of 505 F/g at 2 A/g, significantly outperforming pristine NTO (287.9 F/g at 2 A/g). To assess its practical application, an asymmetric supercapacitor (ASC) was assembled using R-NTO-1.2 as the positive electrode and ultralight graphene (ULG) as the negative electrode, which was obtained from Professor Chunhu Chen, National Sun Yat-sen University. The ASC achieved an energy density of 44 Wh/kg at a power density of 1000 W/kg, with an optimal operating voltage of 2.0 V. These results demonstrate that $NaBH_4$ reduction is an effective strategy for enhancing the electrochemical performance of $NiTiO_3$, making it a promising electrode material for next-generation energy storage devices.

Keywords: nickel titanate; graphene; sodium borohydride; oxygen vacancies; reduction; asymmetric supercapacitor





Sustainable Chemistry Focusing on Clean Energy, Good Health, and Well-Being (Thailand-Taiwan) (SC-O-005)

Exploring sulfonamide-modified phytocannabinoids for anti-inflammatory leads: A computational study

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Cyclooxygenase-2 (COX-2) and cannabinoids receptor type 2 (CB2) are key therapeutic targets for inflammation. Phytocannabinoids have been explored as potential alternatives to nonsteroidal anti-inflammatory drugs (NSAIDs) for their medicinal properties. This study employs the tight-binding semiempirical quantum mechanical (SQM) method, GFN2-xTB, to optimize COX–cannabinoid complexes and compute their binding free energies in implicit solvation ($\Delta G_{bind,solv}$). Our results indicate that carboxylic acid derivatives of phytocannabinoids exhibit strong binding affinities for both COX-2 and CB2. To enhance their anti-inflammatory potency, we investigated sulfonamide modifications and compared their $\Delta G_{bind,solv}$ values to celecoxib, a known COX-2 selective NSAID. Notably, CBTA-C2-SO_2NH_2 exhibited a $\Delta G_{bind,solv}$ of −63.85 kcal/mol, with 27.17% of the binding contribution attributed to the sulfonamide group. In addition, these modified analogs demonstrate favorable drug-like properties and predicted oral bioavailability. These findings provide valuable insights into the rational design of cannabinoid-based anti-inflammatory agents.

Keywords: NSAIDs; sulfonamide cannabinoids; COX-2 inhibitors; noncovalent interactions; binding free energy; molecular docking; semiempirical quantum mechanics

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-O-001)

Evaluation of antioxidant, anti-inflammatory and antimicrobial effects of Rohanaekaash Lepaya; Ayurveda herbal medicine

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Antimicrobial resistance is a significant global health challenge, necessitating alternative therapeutic solutions. Rohanaekaash Lepaya, a traditional Unani formulation, is reputed for its antimicrobial, antioxidant, and anti-inflammatory properties. This study evaluated its effectiveness using various scientific methods. Antimicrobial activity was assessed against *Staphylococcus aureus*, *Escherichia coli*, *Bacillus subtilis*, *Pseudomonas aeruginosa*, *Streptococcus pyogenes* and *Proteus mirabilis* using the well diffusion method. Antioxidant properties were analyzed via the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay and Ferric Reducing Ability of Plasma (FRAP) assay, while the Human Red Blood Cell (HRBC) membrane stabilization method was used for anti-inflammatory evaluation. The results demonstrated significant inhibition zones ranging from 9.40 ± 1.22 mm to 12.60 ± 1.97 mm for Dichloromethane (DCM) extract and 9.50 ± 1.20 mm to 11.46 ± 0.98 mm for hexane extract, with DCM exhibiting potent radical scavenging of IC_{50} of 12.56 µg/mL while hexane extract showed moderate activity with an IC_{50} value of 217 µg/mL. Inflammation inhibition was observed at 61.57% for DCM extract, 29.96% for hexane extract and 50.28% for methanol extract at 1 mg/mL concentration. These findings underscore the therapeutic potential of Rohanaekaash Lepaya, positioning it as a promising candidate for the development of novel pharmacological interventions against antimicrobial resistance.

Keywords: antimicrobial resistance; traditional medicine; Rohanaekaash Lepaya; antioxidant activity; anti-inflammatory activity

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-O-002)

Preliminary investigation of *kshara* powder of *Erythrina variegata* used in Ayurveda

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Kshara is an alkaline substance derived from ashes of medicinal plants and minerals, used in Ayurvedic medicines. There are three main categories of *kshara* powders according to the potency as *Tikshana, Madhya,* and *Mridu*. The *Erythrina variegata kshara* was prepared as the method mentioned by Acharya Sushrutha Samhita in 11th chapter of *Sutra Sthana*, *Kshara* powder was evaluated due to its medicinal value, antioxidant, anti-inflammatory and anti-microbial properties. The antioxidant property was assessed using DPPH assay, *Tikshana*-EC_{50} of 161.1 ppm, *Mridu* 206.2 ppm respectively, with compared of EC_{50} of 55.63 ppm - BHT standard. The anti-inflammatory effect was evaluated using the HRBC membrane stabilization method (IC_{50} of *Tikshana* - 443.1 ppm, *Mridu* 240.3 ppm) Further experiments were conducted under total Ash value, pH, acid insolubility, water solubility, moisture content, functional group identification and heavy metal analysis using FTIR and ICPMS, respectively. This research proves that *Erythrina variegata kshara* powders have antioxidant, anti-inflammatory and antimicrobial properties against *Staphylococcus aureus, E-coli, Bacillus subtilis, Streptococcus pyogenes* and *Proteus mirabills* (Inhibition zones ranging from 1.0 ± 1.20 cm to 3.5 ± 0.94 cm). Continuous research is recommended to elucidate the mechanisms and clinical applications of *kshara* powders of *Erythrina variegata* to ensure human usage.

Keywords: *Erythrina*; antioxidant; *kshara*; anti-inflammatory; Ayurveda

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-O-003)

Preparation and bioactivity of indigenous formula used as hair care oil

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Haircare mainly impacts on the appearance of an individual. Hair dyes are personal care products which use to change the hair color. Even though natural products were used in ancient times, current usage of synthetics have become higher. But synthetic products are with lot of chemicals which are harmful. In this study, a hair dyeing oil was formulated and prepared using natural ingredients such as sesame oil, *Eclipta prostrata*, *Barleria prionitis* L., *Gmelina asiatica* L., *Triphala, Pandanus tectorius*, etc. with reference to an Ayurveda book. Here, a decoction of plant materials was mixed with a juice of *Eclipta prostrata*, sesame oil and prepared a 2410 mL of oil and kept for one month. Then oil was evaluated on antioxidant in DPPH method (IC_{50} value 151–200 ppm), anti-inflammatory in HRBC membrane stabilization method (IC_{50} value 249.5–1440 ppm) and organoleptic properties such as color, appearance, sedimentation; pH value, moisture, refractive index, dyeing effect; chemical properties such as acid value, iodine value, peroxide value and heavy metal content. Accordingly, the above analysis ensured the quality of the product. Finally, it was concluded that this product is applicable for human hair and further product developments and clinical trials should be done for commercialization.

Keywords: antioxidant; ayurveda; hair dye; human hair natural product

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-O-004)

Ferritin and ferritin-sfGFP based nanoparticles for metalloenzyme scaffold engineering and characterization of protein modification activity

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Human heavy chain ferritin (Ftn) is a naturally self-assembled nanoparticle composed of 24 monomers. It assembles rapidly into a hollow spherical shape, built around a basic dimer unit. C2 interface of Ftn that can be engineered for metal chelation and enhanced enzymatic activities was previously identified (*J. Am. Chem. Soc.* **2024**, *146*, 33309–33315). This discovered enzymatic activity highlights the potential of Ftn interface engineering for creating diverse protein surfaces and improving metal chelation. The aim of this study was to isolate different super-folder green fluorescent protein (sfGFP)-fused Ftn intermediate nanoparticles (NPs) and to characterize their structures, novel surfaces, metal-chelating sites, and enzymatic activities in protein Michael addition reactions. Two fusion proteins: sfGFP-Ftn (SFtn) and sfGFP-Ftn-sfGFP (SFtnS) were designed and produced to isolate intermediates at varying temperatures. The purified self-assembled SFtn and SFtnS NPs then accommodated various metals, serving as metalloprotein scaffolds to investigate their enzymatic activities in protein Michael addition, involving a wide range of substrate sizes from 10 to 603 amino acids, as well as for labeling molecules, Michael acceptors.

Keywords: protein nanoparticle; self-assembling engineering; biocatalysis; metalloenzyme design; protein Michael addition

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-O-008)

Potent insulin secretagogues from traditionally used medicinal plants

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The latest International Diabetes Federation (IDF) Diabetes Atlas (2025) reports that 11.1% – or 1 in 9 – of the adult population (2079 years) is living with diabetes, with over 4 in 10 unaware that they have the condition. By 2050, IDF projections show that 1 in 8 adults, approximately 853 million, will be living with diabetes, an increase of 46%. The type 2 diabetes found in the Indian subcontinent is distinct from the more characteristic forms of type 2 diabetes found among Caucasians. In these diabetic subjects relative deficiency in insulin secretion is predominant rather than insulin resistance. Therefore a potent insulin secretagogue will have potential to be a good antidiabetic drug for these type 2 diabetic subjects. We have screened more than 20 traditionally used antidiabetic plants for insulin secretory activity and isolation of pure compounds have been done from most active plants. This presentation will be mainly focused on isolation and structure elucidation of secondary metabolites from four traditionally used antidiabetic plants *Scoparia dulcis* Linn (Chini Jhar), *Zanthoxylum armatum* (Nepali pepper), *Artemisia macrocephala* Jacq. ex Besse, and *Salvia mirzayanii* Rech. f. and their insulin secretary activities on isolated mice islets and pancreatic β-cell line.

Keywords: natural products; diabetes; insulin secretion; *Scoparia dulcis*; *Zanthoxylum armatum*

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-O-010)

Synthesis, *in vitro* and *in silico* evaluation of α-amylase and α-glucosidase inhibitory activities of 2-phenyl-*3H*-quinazoline-4-one derivatives as novel anti-diabetic agents and their kinetic activities

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Chronic hyperglycemia is commonly managed by inhibiting carbohydrate-hydrolyzing enzymes such as α-amylase and α-glucosidase. This study focuses on the synthesis, and evaluation of four para-substituted 2-phenyl-*3H*-quinazoline-4-one derivatives as potential enzyme inhibitors. Para-substituted derivatives were synthesized using spectroscopic techniques, including ^{1}H NMR, ^{13}C NMR, FT-IR, and Mass spectroscopy analysis and evaluated for α-amylase and α-glucosidase inhibition, as well as glucose uptake modulation through *in vitro* studies, while their binding interactions were analyzed using *in silico* methods. *In vitro* assays demonstrated that the 2-(4-methoxyphenyl)-*3H*-quinazoline-4-one derivative (C-iii) has notable inhibitory activity against both α-glucosidase and α-amylase, with IC_{50} values of 0.07 ± 0.00 µM and 0.25 ± 0.00 µM, respectively. Glucose uptake activity studies further revealed an IC_{50} value of 450 ± 1.0 µM for 2-(4-hydroxyphenyl)-*3H*-quinazoline-4-one (C-ii), highlighting its potential to modulate glucose metabolism in yeast cells. Kinetic assays demonstrated that all four derivatives act as non-competitive inhibitors, with unchanged K_m values and a significant reduction in V_{max}. Docking results identified C-iii as the most potent α-glucosidase inhibitor (-7.34 kcal/mol, K_i = 4.20 µM) and C-ii as the most potent α-amylase inhibitor (-6.30 kcal/mol, K^i = 24.24 µM). Additionally, C-ii showed a favorable safety profile, including a high oral LD_{50} and minimal toxicity.

Keywords: hyperglycemia; inhibitory activity; *in silico* activity; *in vitro* activity; glucose uptake

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-O-020)

Growth inhibition of aflatoxigenic *Aspergillus* spp. in stored rice by cinnamon bark oil-chitosan microcapsules and detection of aflatoxins in untreated rice by thin layer chromatography

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Fungal infestations in stored rice pose serious health risks, primarily due to *Aspergillus* spp., which produce toxic aflatoxins. This study explores cinnamon bark oil (CBO) encapsulated in chitosan microcapsules (CBO-CS-MCs) as a natural alternative to synthetic fungicides for inhibiting aflatoxigenic *Aspergillus* spp. Microencapsulation enhances CBO's stability and bioavailability, mitigating its volatility and short shelf life. Using an optimized ionotropic gelation method, the best formulation (3% chitosan, 3 g CBO, 1% STPP) achieved 85% encapsulation efficiency and 16.5% loading capacity. Microscopic and SEM imaging confirmed spherical morphology with crimpled surfaces, and particle sizes between 100–1000 nm. *Aspergillus* spp. isolated from stored rice were cultured on potato dextrose agar and treated with CBO-CS-MCs, determining minimum inhibitory (MID) and minimum lethal (MLD) doses at 6 mg and 14 mg, respectively. Rice grains treated with MLD of CBO-CS-MCs were monitored for three months, showing significantly reduced fungal colony counts and spore densities, reaching the lowest values of 5.33 CFU/mL and 1.26×10^{-4} spores/mL. Thin-layer chromatography using ethyl acetate and dichloromethane (1:1 v/v) mobile phase, effectively detected aflatoxins in untreated rice. This study highlights microencapsulated CBO as a sustainable antifungal agent and demonstrates TLC as a reliable aflatoxin monitoring method.

Keywords: aflatoxin; *Aspergillus* spp.; chitosan; cinnamon bark oil; encapsulation

POSTER ABSTRACTS

Analytical Chemistry (AC-P-003)

Homogeneity and stability of in-house reference material for proximate analysis using chicken feed

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Reference materials are essential for ensuring the accuracy and reliability of analytical measurements. Different properties of reference material need to be examined to ensure they fit their purpose. While certified reference materials undergo a rigorous and costly certification process, in-house reference materials provide a practical alternative with a less stringent approach while still maintaining reliability by adhering to ISO Guide 80. This study evaluated chicken feed as an in-house reference material for proximate analysis, focusing on its homogeneity and stability. Based on the results of homogeneity testing, the chicken feed can be used as an in-house reference material. The study also showed how long the chicken feed can be used as an in-house reference material based on the results of their stability tests. The findings revealed that the chicken feed can be used for 12 weeks for analysis focused on the moisture content. Conversely, for the other parameters such as ash content, crude protein, crude fat, and crude fiber, the in-house reference material can be used for 57 weeks.

Keywords: chicken feed; homogeneity; proximate analysis; reference material; stability

Analytical Chemistry (AC-P-011)

Green synthesis of silver nanoparticles using apricot kernel and assessment of their cytotoxic and genotoxic effects

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The environmental implications and threats of nanoparticles used in different technologies are a significant issue due to uncertainty around their harmful effects on aquatic environments. In this study, biogenic silver nanoparticles were synthesized from *Prunus armeniaca* using a biogenic process and material's genotoxic effects were investigated in aquatic model organism. Acute/chronic toxicity experiments were performed using the method suggested by OECD (Organization for Economic Cooperation and Development) 202–212 guidelines. *Daphnia magna* was subjected to the biogenic silver nanoparticles produced from *Prunus armeniaca* at the different concentrations ranging between 0.09–0.315 mg/L for 96 h. At the end of the 96 h period, the LC_{50} (lethal concentration- at which 50% of cells) value of the biogenic silver nanoparticles was determined to be 0.189 mg/L using probit analysis. Afterwards, cytotoxicity and genotoxicity studies of the biogenic synthesized nanoparticles were carried out for the toxicological assessments of sublethal concentrations of biogenic silver. As a result, the achievements of this work are helpful for understanding the toxicity of biosynthesized to biogenic silver nanoparticles produced from *Prunus armeniaca* to applying crustacean *D. magna.*

Keywords: biogenic synthesis; nanotoxicity; DNA damage; cell viability

Analytical Chemistry (AC-P-012)

Removal of cobalt ions from environmental samples by using nickel-sulfur based nanomaterial

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Cobalt is known as an important cofactor for the optimal functioning of the brain and neurological system, in addition to being necessary for blood production [*J. Mol. Liq.* **2020**, *298*, 112035]. This element, a prevalent toxic metal, is found in the wastewater of nuclear power plants and various industries [*J. Hazard. Mater.* **2009**, *166*, 925–930]. Nevertheless, elevated levels of cobalt can lead to several health issues, including hypotension, pulmonary irritations, paralysis, diarrhea, and skeletal abnormalities, and may even induce mutations in living cells [*J. Hazard. Mater.* **2014**, *270*, 1–10]. The accurate removal of cobalt is crucial for safeguarding food and environmental safety. This study devised a precursor method utilizing nickel-sulfur based nanomaterials to remove cobalt ions from environmental samples. In order to determine the efficiency of the nickel-sulfur based nanomaterials, flame atomic absorption spectrophotometry was used, and the difference of cobalt concentration between influent and effluent solutions were determined in absorbance measurements. The removal efficiency and applicability of the method were optimized by adjusting various experimental parameters through a univariate optimization approach. Interactions between nanomaterials and analytes facilitate adsorption processes, including reduction, electrostatic attraction, co-precipitation, ligand exchange, and chelation, which collectively contribute to potential removal mechanisms [*Water* **2021**, *13*, 1843]. The isotherm and kinetic studies were utilized by using environmental samples. The results demonstrate that the method is both feasible and reliable for removal of cobalt ions in environmental samples.

Keywords: removal; cobalt ions; nickel-sulfur based nanomaterial; environmental samples

Analytical Chemistry (AC-P-014)

An efficient solid phase extraction strategy for the removal of heavy metals from wastewater by utilizing a hydroxyapatite-chitosan-magnetite nanocomposite

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The removal of heavy metals from wastewater to resources including soil, flora, and aquatic environments poses a significant threat to the health of all living species. Consequently, efficient removal approaches are crucial to alleviating the dangers linked to heavy metal pollution in wastewater. Magnetic nanocomposites are regarded as effective agents for the extraction of heavy metal ions, exhibiting significant tunability through various combinations. Their primary limitation, which is reduced efficacy due to aggregation in solutions, can be mitigated by stabilizing the surfaces with a support medium, such as polymeric particles. This work involves the synthesis of hydroxyapatite (HA, $Ca_{10}(PO_4)_6(OH)_2$) nanoparticles using discarded mussel shells obtained from local sellers in İstanbul. Hydroxyapatite was combined with chitosan and Fe_3O_4 nanoparticles to enhance stability and introduce ferromagnetism. The HA nanoparticles and the nanocomposite particles were characterized using X-ray diffraction and scanning electron microscopy. The synthesized nanocomposite was utilized as a dispersive solid-phase adsorbent for separation of heavy metal ions from real wastewater samples. The procedure was meticulously refined by examining several experimental factors on removal effectiveness such as pH, nanosorbent mass, mixing mode, and duration. The improved process presents a straightforward, and efficient method for the removal of heavy metals from wastewater.

Keywords: hydroxyapatite; magnetic nanocomposite; wastewater treatment; heavy metal removal

Analytical Chemistry (AC-P-015)

Determination of formaldehyde in fresh seafood from Cambodia's local market

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Seafood is a highly nutritious food with numerous essential components including proteins, minerals, and vitamins. In contrast, formaldehyde or formalin has often been used as a preservative to prolong shelf life and maintain freshness, raising concerns about food safety and public health due to its toxic effects on human health, especially the digestive system. The purpose of this study is to investigate and quantify formaldehyde in fresh seafood from the local markets in Phnom Penh, Cambodia. Three seafood samples such as shrimp, squid, and short mackerel were examined using UV spectrophotometry based on the reaction of Nash's reagent with formaldehyde forming a yellow color product with the absorbance measured at 412 nm. The results illustrated that the formaldehyde concentration in shrimp ranged from 0.174 to 0.134 mg/kg, 3.199 to 0.164 mg/kg in squid, and 0.168 to 0.140 mg/kg in short mackerel. The method had a limit of detection (LOD) of 0.017 mg/kg and a limit of quantification (LOQ) of 0.055 mg/kg. A recovery percentage of more than 95% was achieved, which demonstrated the accuracy of the analytical method. The formalin concentration in each sample was confirmed to be below the maximum limit of 5 mg/kg, as specified by Malaysia's Food Regulation. However, the use of formalin in food is absolutely forbidden in Cambodia for safety concerns. In conclusion, the results emphasize the importance of ongoing monitoring and proper regulation of formaldehyde levels in seafood to guarantee consumer safety.

Keywords: formaldehyde; seafood; UV spectrophotometry; food safety

Analytical Chemistry (AC-P-018)

A simple and effective zinc oxide nanoparticle based dispersive solid phase extraction method for cadmium determination by flame atomic absorption spectrometry

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There are many analytical methods for the determination of cadmium, which is dangerous even at trace levels [*J. Food Compos. Anal.* **2024**, *127*, 105968]. Therefore, an accurate and applicable analytical method called dispersive solid phase extraction – flame atomic absorption spectrometry was proposed for the determination of trace levels of cadmium. A solid phase extraction procedure was developed in which synthesized zinc oxide nanoparticles were used as adsorbents in order to extract cadmium from aqueous solutions. Zinc oxide nanoparticles were prepared by using the zinc acetate, sodium hydroxide and acetic acid. After, optimization studies were carried out with parameters such as adsorbent amount, different buffer solution media, buffer solution volume, mixing type, mixing time, desorption solvent (HNO_3) concentration and amount. LOQ (Limit of quantification) and LOD (Limit of detection) results for the developed system (ZnO-dSPME-FAAS) were found to be 1.4 µg L^{-1} and 0.4 µg L^{-1}, respectively. In addition, applicability/accuracy of the developed system, were performed in wastewater samples by recovery experiments, and % recovery results were calculated in the range of 94.0–110.5%.

Keywords: cadmium; dispersive solid phase extraction; flame atomic absorption spectrometry; wastewater

Analytical Chemistry (AC-P-020)

Determination of Kjeldahl nitrogen contents in rubber by flow injection conductometric method

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Total proteins in natural rubber could be determined by the Kjeldahl method. The rubber sample was digested for conversion of nitrogen compounds to ammonium, then distilled and analyzed for Kjeldahl nitrogen content by titration. This work developed a simple flow injection conductometric system incorporating with a gas diffusion unit to separate ammonia from the sample matrices. Specially designed flow through cell and an amplifier circuit improved the conductometric detection sensitivity. The system employing a plumbing Teflon tape as a diffusion membrane and without thermostat bath provided a linear calibration graph in range of 1.0-10.0 mg L^{-1} N-NH_4 with a detection limit of 0.44 mg L^{-1}. The relative standard deviation for 11 replicates injections of 5 mg L^{-1} N-NH_4 was 1.70%. According to the paired t-test at 95% confidence level, the results from both the methods were not significantly different ($t_{tabulated}$ = 2.024, $t_{calculated}$ = 0.0331, n = 20), with 98.42% recovery. Application for determination of Kjeldahl nitrogen in natural rubber was carried out. The proposed system achieved a sample throughput of 35 h^{-1} and used significantly less NaOH (275 mg versus 24 g in the standard Kjeldahl titrimetric method), so it could be an interesting alternative for determining total proteins in natural rubber.

Keywords: flow injection; gas diffusion; ammonium; conductometry; proteins; rubber

Analytical Chemistry (AC-P-021)

A fluorescence biosensor for organophosphorus pesticide detection with a portable fluorescence device-based smartphone

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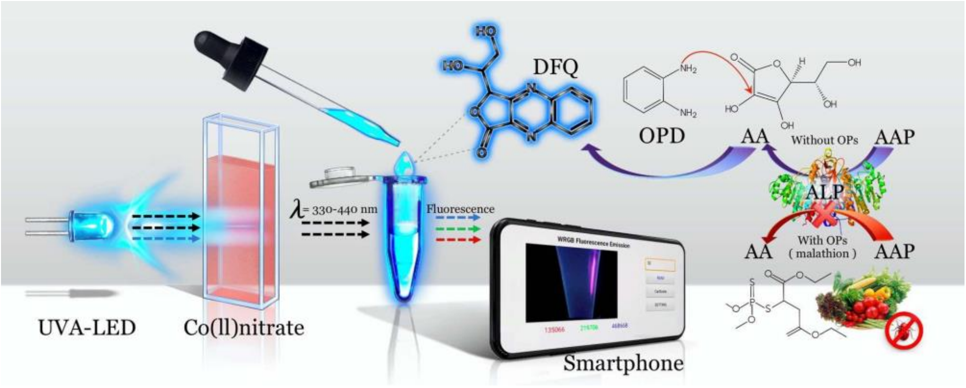
An innovative fluorescence biosensor was successfully developed to detect organophosphorus pesticide (OPs) by utilizing smartphone technology. The assay relied on the enzymatic activity of alkaline phosphatase (ALP), which facilitated the conversion of L-ascorbic acid 2-phosphate sesquimagnesium salt hydrate (AAP) into L-ascorbic acid (AA). The generated AA then reacted with *o*-phenylenediamine (OPD) to yield a fluorescent marker identified as 3-(1,2-dihydroxyethyl)furo[3,4-b]quinoxalin-1(3*H*)-one (DFQ). A novel bandpass approach was developed for a smartphone integrated with a customized portable fluorescence device to measure DFQ fluorescence emission. The device has a unique application that converts the fluorescence intensity into an RGB signal. Malathion was chosen as a representative OP, and its presence inhibited ALP enzymatic activity; the enzymatic activity of the ALP was inhibited, resulting in a decrease in fluorescence intensity, which was proportional to the concentration of malathion. Smartphones can be used to measure fluorescence emission, offering a calibration sensitivity more than 70 times higher than that of conventional spectrofluorometer. The new method can detect malathion in the 0.1–1 ppm range, with a limit of 0.05 ppm. It offers portability, accuracy, and high sensitivity for detecting trace amounts of OPs.

Keywords: organophosphorus pesticide; fluorescence biosensor; smartphone technology



Analytical Chemistry (AC-P-023)

Development of an optical sensor for determination of total antioxidant capacity in food samples

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Antioxidant compounds mitigate oxidative damages by eliminating reactive species through various mechanisms. Recently, modifying existing methods for antioxidant determination and transforming them into practical measurement platforms has gained significant interest [*J. Agric. Food Chem.* **2013**, *61*, 8381–8388]. In this study, the initial steps for developing a microplate-based optical sensor for antioxidant capacity determination were performed using the Cupric Reducing Antioxidant Capacity (CUPRAC) method. The chromogenic oxidation reagent of the CUPRAC method (copper(II)-neocuproine (Cu(II)-Nc)) was lyophilized onto a microplate. After lyophilization, its reactivity toward antioxidants was examined, and in the presence of antioxidants, the absorbance at 450 nm was measured due to the formation of the colored Cu(I)-Nc chelate. The calibration graph of trolox (TR) was linear with a slope of 1.39×10^{3} L mol^{-1} mm^{-1}. This preliminary study presents a practical method with advantages such as low sample consumption, on-site analysis capability, and simultaneous multi-sample analysis. Upon completion, this approach holds potential for adaptation into a kit format for future applications.

Keywords: antioxidants; optic sensors; CUPRAC; microplate

Analytical Chemistry (AC-P-024)

Application of electrochemical sensor based on biomass-derived carbon composites electrode for simultaneous determination of cadmium and lead

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In this work, carbon-based materials prepared from biomass were mixed with carbon black to modify the surface of a screen-printed electrode. This modification enhanced the electrode's electrical conductivity and surface area. The developed electrochemical sensor demonstrated high sensitivity and ease of use for the simultaneous determination of trace cadmium and lead. The sensor provided the best performances at a low working potential of -1.2 V (vs. Ag/AgCl) using differential pulse voltammetry (DPV). The limit of detection (LOD) and limit of quantitation (LOQ) were determined based on 5 and 10 of cadmium and lead, respectively. Non-metallic materials, such as concrete roofing tiles, can incorporate metal ions, which are considered to pose a risk to public health. Therefore, their presence is restricted to permitted levels. In Thailand, the maximum allowable concentration should not exceed 10 µg/L for cadmium and 50 µg/L for lead, according to Thai Industrial Standard (TIS) 535-2556. The developed sensor was further applied to analyze real samples, providing an alternative to standard methods such as atomic absorption spectrometry or inductively coupled plasma. It was found that the developed sensor can be used to detect these metals within the acceptable range set by the TIS criteria.

Keywords: biomass-derived carbon; cadmium; heavy metal; electrochemical sensor; lead; TIS 535-2556

Analytical Chemistry (AC-P-026)

Determination of cadmium in ceylon tea matrices by preconcentration with magnesium aluminum oxide nanoparticle before flame atomic absorption spectrometry

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Cadmium (Cd) is one of the most hazardous heavy metals, and its accumulation in human kidneys and liver causes significant harm to the urinary and DNA repair mechanisms, potentially leading to lung and prostate cancer [*Microchem. J.* **2021**, 164]. Therefore, the development of techniques for cadmium detection is crucial because of the element's significance in the environment and toxicology [*Environ. Monit. Assess.* **2017**, *189*, 9]. In this study, an analytical method was developed to determine low levels of cadmium by flame atomic absorption spectrometry at low levels in Ceylon tea matrices using dispersive solid-phase extraction with magnesium aluminum oxide ($MgAl_2O_4$) as an adsorbent. For this purpose, $MgAl_2O_4$-NPs were synthesized using the sol-gel method combined with the calcination procedure and characterized using scanning electron microscopy (SEM) and X-ray diffraction (XRD) systems. Several parameters affecting the extraction efficiency, such as nanoparticle amount, sample volume, buffer solution pH, buffer volume, eluent concentration, mixing type, and period, were optimized. The analytical performance of the proposed system was then evaluated under optimal conditions.

Keywords: cadmium; $MgAl_2O_4$ nanoparticle; dispersive solid phase microextraction; flame atomic absorption spectrometry

Analytical Chemistry (AC-P-028)

Removal of nickel ions from artificial wastewater samples by using copper(II) phosphate based nanoflowers assisted adsorption based treatment strategy

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The emergence of nanotechnology signifies a substantial transformation in the advancement of materials utilized for adsorbent synthesis. This technology enables the modification of materials at the molecular level, resulting in enhanced efficiency in pollutant capture [*Heliyon* **2024**, *10*, e29573]. Adsorption-based strategies are crucial for maximizing the efficiency of nanoparticles in wastewater treatment, offering a highly effective, versatile, and sustainable solution to several complex challenges associated with water pollution [*ChemistrySelect* **2024**, *9*, 25]. In this study, a new and easy co-precipitation method was proposed to remove nickel ions (Ni^{2+}) from aqueous solution by using copper nanoflowers having petal-like morphology. Univariate optimization measurements were carried out to maximize the removal efficiency. Ni was determined with the help of flame atomic absorption spectrometry (FAAS). Spiking tests were carried out on artificial wastewater samples. After spiking Ni^{2+} from wastewater with 50, 25, and 10 mg/L Ni^{2+}, satisfactory results of 82.6±1.8%, 91.4±2.0%, and 94.8±3.6% were obtained, respectively. These outcomes demonstrate the suggested method's accuracy and applicability in eliminating Ni^{2+} from wastewater [*Anal. Lett.* **2024**, *57*, 6].

Keywords: nickel ions; adsorption; copper(II) nanoflowers; wastewater

Analytical Chemistry (AC-P-030)

Determination of cyanide with biogenically produced AuNP

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Cyanide (CN^-) is an extremely harmful anion known for its ability to accumulate in water, soil and air, and poses crucial risks to organisms even in trace structures. Therefore, it is essential to use accurate and sensitive analytical methods to determine any of the cyanide. This successful, simple, and effective therapeutic method for the quantitative determination of cyanide by UV-Vis spectrophotometry via gold nanoparticle (AuNP) solutions synthesized with rosehip extract has been developed. Gold nanoparticles are frequently used as promising tool in the determination of various organic and inorganic products. In this study, gold nanoparticles were prepared using auric acid containing citrate as a stabilizer. The reduction reaction occurred by using rosehip extract instead of harmful chemicals UV-Vis absorption spectra revealed that the communication between cyanide ions and AuNPs resulted in meaningful decreases in the absorption peak of the SPR (surface plasmon resonance) band at 524 nm. The presented colorimetric sensor exhibited an outstanding detection performance for cyanide ions in the range of 2.0 to 20 mg/L. The limit of detection (LOD) was determined as 4.93 mg/L and the limit of quantification (LOQ) as 16.42 mg/L. In addition, the proposed colorimetric method was successfully applied to different soil samples, thus demonstrating its practical potential.

Keywords: AuNP synthesis; biogenic method; determination of cyanide; colorimetric sensor; SPR

Analytical Chemistry (AC-P-031)

$ZnCo_2O_4$ nanoparticles based dispersive solid phase extraction method for the preconcentration of indium prior to flame atomic absorption spectrophotometry measurements

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A heavy-metal element indium is widely used in a variety of fields, such as biomedicine, alloys, and semi-conductors. As the amount of indium released into the environment is significantly rising as a result of the gradually increasing indium use, the risk of indium pollution tends to increase in tandem. Furthermore, it has been established that indium compounds have a certain level of toxicity, and cause several health problems, particularly those related to dental decay, joint discomfort, and the germinal and inherit system if income levels rise above a specific threshold [*Microchem. J.* **2018**, *137*, 266–271]. Consequently, the development of an analytical method for the determination of trace level indium in industrial effluents and environmental water is a sensible way to avoid indium pollution. In this research, $ZnCo_2O_4$ nanoparticles were used for indium determination in the method based on dispersive solid phase extraction (DSPE) before flame atomic absorption spectrometry (FAAS) measurement. For the optimum parameters, all variants (pH solution, buffer solution volume, $ZnCo_2O_4$ nanoparticles amount, mixing type and period, and eluent volume and concentration) were optimized for increasing the sensitivity in detection of FAAS instrument. The linear working range, coefficient of determination (R^2), and limit of detection/quantification (LOD/LOQ) of the outlined approach were assessed using system analytical performance experiments. Following that, recovery studies using environmental samples were conducted to determine the applicability and accuracy of the suggested method.

Keywords: indium; dispersive solid phase extraction; FAAS; $ZnCo_2O_4$ nanoparticles

Analytical Chemistry (AC-P-033)

Emulsion liquid membrane with nanocellulose semicrystals from tabah bamboo (*Gigantochloa nigrociliata*) as separation media for methylene blue

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Dye waste is one of the pollutants produced by the textile industry and can contaminate water sources around industrial sites if the waste treatment process is inefficient. In this study, the extraction efficiency of methylene blue in wastewater was investigated using the bioemulsion liquid membrane (Bio-ELM) technique, modified with semicrystalline nanocellulose (CNC) derived from tabah bamboo. The CNC was produced by preparing tabah bamboo samples into cellulose powder, and hydrolyzed with 55% H_2SO_4 to produce CNC. The liquid membrane was prepared using nanocellulose crystals 3% as impregnated adsorbents; span 80 as a surfactant, *n*-heptane as a carrier, and palm oil (2:2:96), and NaOH 0.25 M as the membrane and internal phases, respectively. The extraction percentage was analyzed by measuring the methylene blue with the initial concentration of 20 mg/L in the external phase using the UV-Vis spectrophotometry method, and the effect of nanocellulose crystal concentration was observed. The results showed that 99.36±0.08% of methylene blue was successfully extracted using nanocellulose crystal 3,0% w/v. Therefore, it can be concluded that nanocellulose crystals can be used as biomaterial components of liquid membranes in methylene blue wastewater treatment, particularly in the Bio-ELM process for re-extraction.

Keywords: bioemulsion liquid membrane; cellulose nanocrystal; methylene blue; palm oil; tabah bamboo

Analytical Chemistry (AC-P-034)

Triple-multivalent aptamer-tetrahedral DNA nanostructure for enhanced signal amplification and rapid mercury ion detection

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DNA nanostructures are emerging as promising biosensing platforms due to their programmability, predictable assembly, and compatibility with aptamers for enhanced selectivity. Triple-multivalent aptamers (tApt) integrated with tetrahedral DNA nanostructures (TDN) offer improved biosensing performance due to their high affinity and selective binding. This study presents a tApt-based aptasensor immobilized on TDN and interfaced with an electrochemically reduced graphene oxide (ERGO) electrode for mercury ion (Hg^{2+}) detection [*Biosen. Bioelectron.* **2024**, *249*, 116039]. Compared to a linear aptamer-modified electrode (sApt/ERGO-GCE), the 3D tApt/ERGO-GCE sensor exhibits superior sensitivity and signal amplification, achieving an unprecedented limit of detection (LOD) of 4.1 zM, significantly lower than the 0.71 fM LOD of sApt/ERGO-GCE. Additionally, the tApt/ERGO-GCE sensor demonstrates a faster half-saturation time ($T_{1/2}$) of 6 minutes, highlighting improved reaction kinetics. The enhanced performance is attributed to the tetrahedral structure's rigid framework, which promotes optimal aptamer orientation, increased binding sites, and efficient analyte capture. In contrast, linear aptamers exhibit random orientations, reducing target molecule interaction. Furthermore, dissociation constant (K_d) analysis confirms stronger Hg^{2+} binding in the tApt system. This study highlights the potential of tApt-based tetrahedral DNA nanostructures as a powerful platform for ultrasensitive and rapid biosensing applications.

Keywords: triple multivalent aptamer; tetrahedron structure; dissociation constant; mercury ion; electrochemically reduced graphene oxide

Analytical Chemistry (AC-P-035)

Unlocking the power of chirality: Surface nanoarchitectonics of halloysite nanotubes for enantioselective recognition

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Developing cost-effective electrode materials with high efficiency for enantioselective recognition has gained considerable interest. In this work, we take advantage of the physicochemical properties of halloysite nanotubes (HNTs) to use them as electrode substrates for the enantiorecognition of chiral probes guided by inherently chiral oligomers-based thiophene. The HNTs were modified with an enantiopure 3,3'-dibenzothiophene derivative, oligo-(3,3'-dibenzothiophene) (BT_2T_4) by chemical oligomerization in the presence of a potent oxidant agent. With this composite (oligo-*(S)*-BT_2T_4@HNTs and oligo-*(R)*-BT_2T_4@HNTs), a differentiation in terms of peak potential (560-650 mV) between the two antipodes of L- or D-3, 4-dihydroxyphenylalanine (L- or D-DOPA), chosen as a model chiral analyte, was observed. This differentiation is attributed to favorable or unfavorable diastereomeric interactions between the inherently chiral oligomer and the antipode of the chiral molecule. Interestingly, such a modified electrode showed an outstanding range of quantification (R^2 = 0.977–0.996) and reproducibility. The results display the perspective of using HNTs modified electrodes as a new class of chiral device, opening up potential applications in the field of enantioselective recognition.

Keywords: halloysite nanotubes; inherently chiral oligomers; chirality; analytical probes; enantioselective recognition

Analytical Chemistry (AC-P-037)

Chiral separation of emtricitabine and its epimers and enantiomers using LC-MS/MS method development and optimization

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Emtricitabine is a widely used antiviral drug, and its chiral purity is critical due to potential differences in the pharmacological effects of its stereoisomers. Separating both its diastereomers and enantiomers is essential for quality control and regulatory compliance. However, existing monographs rely on normal-phase conditions, which are less compatible with routine pharmaceutical analysis. This study systematically evaluates various chiral stationary phases under reversed-phase LC conditions and identifies an amylose-based chiral stationary phase as optimal for achieving complete resolution of all four stereoisomers. Mobile phase composition—including buffer type, pH, and organic modifier—was optimized to enhance separation efficiency. The developed method is fully compatible with LC-MS/MS for sensitive detection and can also be implemented on an LC-UV platform, making it suitable for routine use in pharmaceutical manufacturing. The method demonstrated excellent sensitivity, with limits of detection (LOD) for the enantiomer, 5-epimer, emtricitabine, and 2-epimer determined to be 20, 17, 13, and 18 ng/mL, respectively. Corresponding limits of quantification (LOQ) were 60, 50, 38, and 53 ng/mL. The total analysis time was 25 minutes, providing reliable baseline separation and quantification within a practical analytical window. This approach offers a robust and accessible alternative to normal-phase methods, improving ease of adoption in routine drug quality control.

Keywords: emtricitabine; chiral separation; chiral drug; enantiomer; LC-MS/MS

Analytical Chemistry (AC-P-038)

CNT-FET-based bioelectronic sensor mimicking the human endocannabinoid system for cannabinoid detection

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Cannabinoids regulate neuromodulation and physiological processes by interacting with the human endocannabinoid system. Their role in neurodegenerative diseases and brain reward pathways highlights the need for precise monitoring of cannabinoid-receptor interactions to develop therapeutic strategies using agonists and antagonists.

In this study, we present a bioelectronic sensor utilizing a single-walled carbon nanotube field-effect transistor (swCNT-FET) to mimic the human endocannabinoid system for real-time electrical analysis [*Biosen. Bioelectron.* **2024**, *264*, 116686]. Human cannabinoid receptor 1 (hCB1R) was incorporated into nanodiscs (NDs) and immobilized onto the CNT-FET surface, forming a highly sensitive platform for ligand detection.

This system detected the cannabinoid ligand anandamide (AEA) at concentrations as low as 1 fM with exceptional selectivity and responsiveness. It also identified the hCB1R agonist Δ^9-tetrahydrocannabinol, while the antagonist rimonabant significantly reduced the AEA-induced signal, confirming its potential for receptor modulation studies.

Our CNT-FET-based bioelectronic sensor enables label-free, high-sensitivity analysis of cannabinoid interactions, offering a promising tool for pharmacological research and drug discovery.

Keywords: bioelectronic sensor; CNT-FET; human endocannabinoid; cannabinoid

Analytical Chemistry (AC-P-039)

Development of a simple spectrophotometric system for detection of sodium ion

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The detection and quantification of sodium ions (Na^+) in various samples are essential in numerous fields, including environmental monitoring, clinical diagnostics, and industrial processes. Traditional methods for sodium ion detection, such as ion-selective electrodes (ISEs) and flame photometry, often require specialized equipment, skilled operators, and are limited by factors such as high cost and the need for continuous calibration. This research focuses on developing a simple, cost-effective spectrophotometric system for detecting sodium ions (Na^+) in aqueous solutions. The system detects sodium through the formation of a white precipitate upon reaction with potassium antimony(III) hydroxide ($K[Sb(OH)_6]$), which correlates with the sodium concentration. The presence of this precipitate is quantified using a Light Dependent Resistor (LDR), offering a low-cost alternative to traditional techniques. The working range of the system spans from 0.02 to 0.18 M sodium concentration, with the white precipitate forming at the bottom of the container. Detection limit and correlation coefficient are 0.01 M and 0.993, respectively. The state of the reagents, including the sample cell used for detection, was investigated. Interference effects will be further studied. A portable and user-friendly system suitable for use in various practical applications, such as water quality monitoring, clinical diagnostics, and food industry analysis.

Keywords: sodium ion detection; light dependent resistor (LDR); simple spectrophotometry

Analytical Chemistry (AC-P-045)

An electrochemical paper-based immunosensor for the dual detection of oxytetracycline and enrofloxacin

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Antibiotic resistance poses a significant global threat, with the widespread use of antibiotics such as oxytetracycline (OTC) and enrofloxacin (ENR) in aquaculture contributing to environmental contamination and ecological imbalance. In this study, a dual electrochemical immunosensor based on a paper-based analytical device (ePAD) was developed for the simultaneous, label-free detection of OTC and ENR residues. The sensor was fabricated by modifying a screen-printed graphene electrode (SPGE) with copper(II) phthalocyanine (CuPc) and amine-functionalized nanosilica (NH_2-SiO_2), which enhanced the electrochemical response and facilitated effective antibody immobilization. The NH_2-SiO_2 acted as a scaffold for the selective attachment of antibodies, ensuring high specificity toward both OTC and ENR. Ferri/ferrocyanide was used as the redox probe to monitor the immunosensor response. Differential pulse voltammetry (DPV) was employed for quantitative detection, yielding a linear range of 1–200 ng mL^{-1} with low detection limits of 0.80 ng mL^{-1} for OTC and 0.58 ng mL^{-1} for ENR under optimized conditions. The proposed dual-sensing platform exhibited excellent sensitivity, selectivity, and reproducibility. Moreover, its portability, disposability, and user-friendly operation make it a promising alternative for on-site monitoring of antibiotic residues in food and environmental samples. This work underscores the potential of ePAD-based immunosensors for rapid and cost-effective food safety applications.

Keywords: electrochemical immunosensor; dual detection; paper-based analytical device; oxytetracycline; enrofloxacin

Study on the conversion of residual lithium titanate oxide into lithium ion sieve adsorbents

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Lithium is a critical metal in the new energy industry. Compared to traditional lithium mining, lithium extraction from brine has a lower environmental impact, with lithium adsorbents playing a central role in direct lithium extraction (DLE) technology. Given that lithium titanate oxide (LTO) exhibits excellent stability in acidic environments and has a low dissolution rate, this study develops lithium ion sieves using residual LTO from battery manufacturing and synthetic LTO. The effects of different acid leaching conditions, including hydrochloric acid concentrations (0.1 M–0.4 M), leaching time (6–48 hours), and solid-to-liquid ratios (2 g/L–8 g/L), on lithium removal efficiency were investigated. Further, the adsorption performance for lithium solution and brine was evaluated. XRD analysis showed recycled LTO has a spinel structure, while synthetic LTO is layered. Adsorption tests using a pure lithium solution revealed capacities of 8 mg/g (recycled LTO) and 23 mg/g (synthetic LTO). Layered-type adsorbents generally outperform spinel-type due to their open interlayer spacing, which enhances lithium ion accommodation. This study also explores adsorption in low-concentration lithium solutions and salt-production brine. By optimizing adsorption conditions, this research aims to develop more efficient and stable lithium adsorbents, offering a sustainable strategy for lithium recovery from brine.

Keywords: lithium ion sieves; brine; adsorption; residual lithium titanate oxide (LTO)

Chemistry for Energy and Environment (CE-P-030)

Utilizing waste-based inhibitors to prevent PCDD/F formation during the valorization of solid recovered fuel from paper mill waste rejects

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Polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) are significant concerns in combustion processes due to their extreme toxicity, environmental persistence, and potential for bioaccumulation. These compounds form unintentionally during the incomplete combustion of organic materials containing chlorine, such as medical waste, biomass, or industrial materials. The combustion of paper mill waste for energy recovery raises concerns regarding PCDD/Fs emissions primarily due to its high plastic content and associated elevated chlorine levels. This study examines the effectiveness of waste-based inhibitors in mitigating PCDD/F emissions during the combustion of solid recovered fuel (SRF) derived from plastic reject waste generated by a paper mill. Thermal treatment experiments were conducted using a laboratory furnace at 350 °C for 30 minutes. SRF derived from plastic reject waste generated by a paper mill was blended with 2 wt% of either polyurethane foam (PUF) or clam shells (CS). Ash samples were collected following combustion to assess the inhibitory performance of each inhibitor. To evaluate the effect on flue gas emissions, a dedicated thermal setup was employed, capable of capturing PCDD/Fs in both gaseous and particulate phases using a PUF+XAD-2 resin sandwich and a quartz fiber filter, respectively. Based on initial screening, more effective inhibitor was further tested at higher concentrations (5%, 10%, and 25%) under thermal treatment at 400 °C for 30 minutes. For chemical analysis, PCDD/Fs retained in the filters and PUFs were extracted using toluene in a Soxhlet apparatus. The extracts were then concentrated and purified using concentrated sulfuric acid. Quantification of PCDD/Fs was performed using a high-resolution gas chromatograph coupled with a high-resolution mass spectrometer (HRGC/HRMS). The HRGC (Hewlett–Packard 6970 Series, CA) was equipped with a silica capillary column (J&W Scientific, CA) and a splitless injector, while detection was carried out using a Micromass Autospec Ultima HRMS (Manchester, UK). PUF demonstrated exceptional suppression, achieving over 90% efficiency across all tested ratios and up to 99.9% mass and TEQ inhibition at 10% addition. CS showed limited effectiveness, with mass and TEQ reductions of 13.3–14.5% and 29.3–42.4%, respectively, due to its high decomposition temperature. Flue gas tests confirmed PUF's effectiveness, reducing PCDD/F emissions by 62.1–96.5% in flue gas and 60.9–96.7% in ash, with 25% addition as the highest. Thermogravimetric analysis coupled with gas chromatography–mass spectrometry (TGA-GC/MS) revealed that PUF thermally decomposes into various nitrogen-containing species, eventually forming ammonia. Ammonia may inhibit PCDD/F formation through multiple mechanisms: (i) inactivation of catalytic metals by interacting with copper compounds (e.g., CuCl, $CuCl_2$), leading to the formation of less active or inert complexes; and (ii) chlorine consumption via reactions with chlorine species (e.g., Cl_2), resulting in the formation of NH_4Cl or chlorinated amines. These pathways reduce the availability of free chlorine, thereby limiting the chlorination of aromatic precursors and ultimately suppressing PCDD/F synthesis. These results highlight PUF as a promising waste-based inhibitor for cleaner energy production, offering a sustainable and cost-effective solution for mitigating PCDD/F emissions in waste-to-energy applications.

Keywords: PCDD/F, waste-based inhibitor, solid recovered fuel, paper mill

Chemistry for Energy and Environment (CE-P-032)

Synthesis of magnetic-Ag-biochar derived from corn husk for removal pollutant organic compounds and antibacterial activity against *Escherichia coli*

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Corn husk (CH) was used to create the multifunctional magnetic-silver/biochar material (M-Ag/CHB). A magnetic corn husk biochar containing colloidal Fe_2O_3 particles embedded inside a porous biochar matrix was synthesized by the thermal pyrolysis of $FeCl_3$-treated biomass. The manufacture of magnetic silver-biochar material utilizes $AgNO_3$ solution as the silver supply and polyphenol derived from green tea as the reducing agent. Their structure and morphology were analyzed using X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET) specific surface area measurements, Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The findings demonstrated that the magnetic-silver nanoparticles were effectively incorporated onto the biochar. The adsorption effectiveness of these materials exhibited a superior removal of methylene blue (~90%) in contrast to methyl red (~ 70%). The M/CHB and M-Ag/CHB exhibited a superior adsorption ability for methyl red compared to CHB and Ag/CHB due to the presence of Fe_2O_3 loading. Their antibacterial efficacy against Escherichia coli (*E. coli*) was assessed using the tablet colony counting technique and the optical density (OD) method. The findings suggested that the magnetic-silver-biochar composites exhibited more efficacy and enhanced antibacterial performance compared to the original biochar, suggesting promising applications for these composites in the antibacterial domain.

Keywords: magnetic-silver-biochar; corn husk; pollutant organic compound; *Escherichia coli*

Chemistry for Energy and Environment (CE-P-036)

Flexible supercapacitors based on cellulose nanofibers from banana peels with MXene as conductive substrate and polyaniline as conductive polymer

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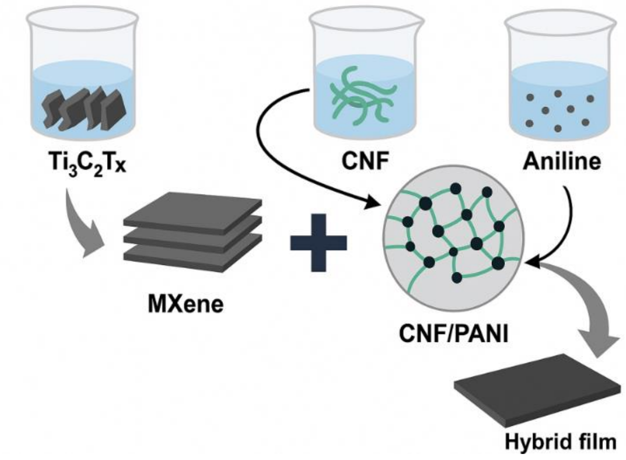
This study presents the synthesis and characterization of flexible supercapacitors based on MXene electrodes reinforced with cellulose nanofibers (CNF) extracted from banana peels, and polyaniline (PANI) as a conductive polymer. CNF was obtained through alkali treatment, bleaching, acid hydrolysis, and sonication. MXene was synthesized by acid etching. The electrodes were prepared using an insertion technique, followed by vacuum filtration and in-situ polymerization of PANI, forming a porous, layered aerogel structure that enhances the integration of all components. Characterization was conducted using Scanning Electron Microscopy (SEM) to observe surface morphology, X-ray Diffraction (XRD) to examine the crystalline structure, and Fourier Transform Infrared Spectroscopy (FTIR) to identify functional groups. Electrochemical performance was evaluated through cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). These tests were used to assess specific capacitance, charge-discharge behavior, internal resistance, and long-term cycling stability. The addition of PANI improves charge storage through redox activity and enhances electrical conductivity. The integration of MXene, bio-derived CNF, and PANI demonstrates a promising approach for the development of efficient, sustainable, and environmentally friendly supercapacitors with high energy performance, making them suitable for future energy storage applications.

Keywords: flexible supercapacitor; MXene; cellulose nanofiber; polyaniline



Food, Agriculture, and Cosmetics (FA-P-010)

Carbohydrate content test of tofu liquid waste as an alternative media for the growth of *Streptococcus mutans*

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Alternative media for bacterial growth using liquid tofu waste, the nutrient content in liquid tofu waste has the potential as a source of nutrients for the growth of bacteria. To see the carbohydrate content in tofu liquid waste, qualitative tests (Benedict) and quantitative tests using the DNS method were carried out. The growth of *Streptococcus mutans* isolates alternative media also carried out. The method used is an experimental method with a sampling technique in the form of Purposive Sampling. Qualitative test results were carried out using Benedict method from 8 test samples, 4 positive samples showed the presence of carbohydrates marked by a color change to green. Further quantitative test using the DNS method, test samples with the highest carbohydrate content obtained results at a concentration of 20% (0.006822%), concentration of 50% (0.009983%) and concentration of 80% (0.017919%). Then pH measurements were carried out on the 20% media 5.08, 50% concentration 4.78 and 80% concentration 4.69. *Streptococcus mutans* grew on alternative media of tofu liquid waste concentrations of 20%, 50% and 80%. Concentration of 20% is an effective alternative medium for the growth of *Streptococcus mutans* because the pH of the medium is optimum for the bacteria.

Keywords: benedict; DNS; tofu liquid waste; alternative media; *Streptococcus mutans*

Future in Chemical Education (FE-P-001)

Teaching about acrylamide in food through the interrupted case study method

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Acrylamide can be generated from food components during heat treatment as a result of the Maillard reaction. Acrylamide is a toxic compound and classified as probably carcinogenic to humans in Group 2A by The International Agency for Research on Cancer. Students need to acquire adequate knowledge to enable them to understand and establish connections between the chemical structure of acrylamide and its biological activity, as well as being able to reason critically about the intensity of the response and the effects that this compound can trigger in the body. In this context, case-based learning, which tells stories related to everyday life is an alternative. This work reports the application of interrupted case studies on acrylamide in food, which were implemented in a scientific communication course offered to undergraduate chemistry students. The students developed hypotheses and evaluated data provided in each case study. Results from a Descending Hierarchical Classification Analysis of argumentative texts written on the subject, performed on IRAMUTEQ software, and from a quiz answered by 98% of students in the course, provided evidence for the effectiveness of the case studies to promote knowledge acquisition. CNPq 300448/2025-2.

Keywords: case studies; food chemistry; argumentation; acrylamide

Future in Chemical Education (FE-P-002)

Implementing LDR to assist disabled students in reaction rate practicum

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This study explores the use of a Light Dependent Resistor (LDR) as an assistive tool to enhance accessibility and engagement for students with disabilities in class XI MIPA semester 3 SMAN 1 Bungursari Purwakarta , particularly those with visual impairments, in a reaction rate practicum and is a continuation of the work “Utilization of Light Dependent Resistor as a Tool to Measure the Accuracy of Reaction Time and Reaction rate” which was presented in ICCE 2024. The experiment involved measuring the reaction rate between Sodium thiosulphate and hydrochloric acid using an LDR system. The LDR was employed to detect changes in light intensity caused by color changes in the solution, which were then converted into electrical signals. The methodology included the preparation of tools and materials, system setup, practical implementation of the chemical reaction, and data analysis to evaluate the effectiveness of the LDR system. The LDR system successfully detected changes in light intensity corresponding to the reaction rate, providing accessible feedback to students with visual impairments. inclusive. While the LDR system showed promise, the study was limited to a single chemical reaction (sodium thiosulphate and hydrochloric acid). Further research is needed to test the system's applicability to other reactions and its scalability in diverse educational settings. Additionally, the study did not explore the long-term impact of using LDR technology on students' learning outcomes or the potential challenges of implementing such systems in resource-constrained environments. The findings suggest that LDR technology can be a valuable tool for promoting inclusivity in science education, particularly for students with disabilities.

Keywords: LDR; reaction rate; disabilities; inclusive education; assistive technology

Future in Chemical Education (FE-P-003)

Implementation SSC (Small Scale Chemistry) in the practical work on making carbon dioxide gas from egg shells to improve student creativity in stoichiometry material

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This study aims to apply the small-scale chemistry (SSC) approach in laboratory practice on carbon dioxide (CO_2) production from eggshells to encourage students' creativity in stoichiometry subjects. The SSC approach is suitable for high school level because it uses minimal chemicals, simple equipment, and safe techniques. This type of research is descriptive quantitative. Respondents are students of grade XI IPA who have taken stoichiometry lessons. Student creativity data were collected through observation, interviews, and rubrics then analyzed descriptively quantitatively. Free-range chicken eggs, domestic chicken eggs, and duck eggs were used in the experiment. The findings of the study showed that students' creativity increased when SSC was applied in laboratory practice of making carbon dioxide from eggshells. The use of free-range chicken eggshells produced (an average of 24 mL CO_2) higher than domestic chicken (an average of 20 mL CO_2) and duck eggs (an average of 18 mL CO_2). After practicing using SSC in class, students were able to understand the concept of stoichiometry more effectively. The implementation of the SSC technique practicum has been proven to have an effect on creativity with the results of the pretest (average 78%) and posttest (average 95%) which changed significantly. It is concluded that the implementation of the SSC approach makes teaching students chemistry lessons about stoichiometry more interesting and relevant and increases students' creativity and understanding.

Keywords: small scale chemistry, creativity, stoichiometry, practicum, carbon dioxide gas

Future in Chemical Education (FE-P-006)

Effect of training evaluation on curriculum development and implement in chemical risk management

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Chemical Risk Management (CRM) is a system to control safety and security risks associated with hazardous chemicals. For curriculum development in CRM we must determine more needs such as who's target audiennce, kind of organization , learner'previous knowledge and expertise, these process are called training needs analysis (TNA), It is the basis for building the curriculum and Implement a training course , we must evaluate TNA stage before we go to the Development curriculum stage and doing it at every stage(formative evaluation) to ensure solve mistakes befor become problems. to ensure that, we can Apply (ADDIE)curriculum cycle that includes five stage:

1-Analyze: Determine a target audience who should be knowledgable of CRM and the resources required for the training.
2-Design: Translate all the information collated in the Analyze phase into a learning design.
3-Develop: Teaching materials should be relevant to learning objectives.
4-Implement: All material should be ready and available and educator ready to present a compelling learning experience.
5-Evaluate: Did the target audience find Curriculum relevant to their Training Needs? (summative evaluation). There are two other types of evaluation: Training Impact Assessment and measurement of Return on Investment in Training.

When we evaluated Analyze stage we ensure that target audiennce are Chmestry Teachers and their language is Arabic this led us in Design and Develop stages we must put Use of Personal Protection Equipment in Chmecal laboratories in the Curriculum and translate the cuorse material to Arabic language(evaluate before training) (formative evaluation),in Implement stage we designate approriate staff to observe the training to ensure that the Curriculum and training assistannces is suitable to Training Needs (evaluate During training) (formative evaluation), in Evaluate stage we select evaluation questions to determine strengths and weaknesses in the training cuorse, Did the target audience find Curriculum relevant to their Training Needs? (evaluate After training) (summative evaluation). When we applying the evaluation according to the ADDIE model, we noticed that the Curriculum at was relevant to trainees Training Needs, and weaknesses has been solved before became mistaks, when we comparison summative evaluation rasults and analysis stage that will help improve training in the futur and will help to do Training Impact Assessment and measurement of Return on Investment in Training.

Keywords: training; evaluation; chemical; risk; management

Future in Chemical Education (FE-P-007)

Collaborative learning in chemistry: A case study on perfume creation and ester synthesis among Thai and Korean science high school students

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This study explores collaborative learning in chemistry through perfume branding and ester synthesis among high school students from Thailand and Korea. A total of 17 students from Mahidol Wittayanusorn School in grade 11 and 9 students from a Korean science high school participated. The fundamental concepts of perfumery, including key components, proportions, and common formulations were guided. Students conducted research, collaborated to design their own fragrance and logo, and ultimately presented their perfume brand. Each group explained their scent, its meaning, and the rationale behind their formulation. Assessment results indicate high student engagement and understanding. The average score for comprehension of perfume composition was 4.58, understanding the advantages and disadvantages of synthesized perfumes was 4.46, and knowledge of alcohol's effect on fragrance longevity was 4.38. Additionally, students voted on the most impressive perfume created by their peers. The findings highlight the effectiveness of collaborative learning in enhancing chemistry education and creativity in cosmetic science. This approach not only deepened students' understanding of ester synthesis and fragrance formulation but also fostered teamwork, problem-solving skills, and cross-cultural exchange.

Keywords: collaborative learning; perfume; ester synthesis

Inorganic Chemistry (IC-P-003)

Cd(II) coordination polymers constructed from tris-pyridyl-tris-amide and polycarboxylic acid: Synthesis, structures and sensing properties

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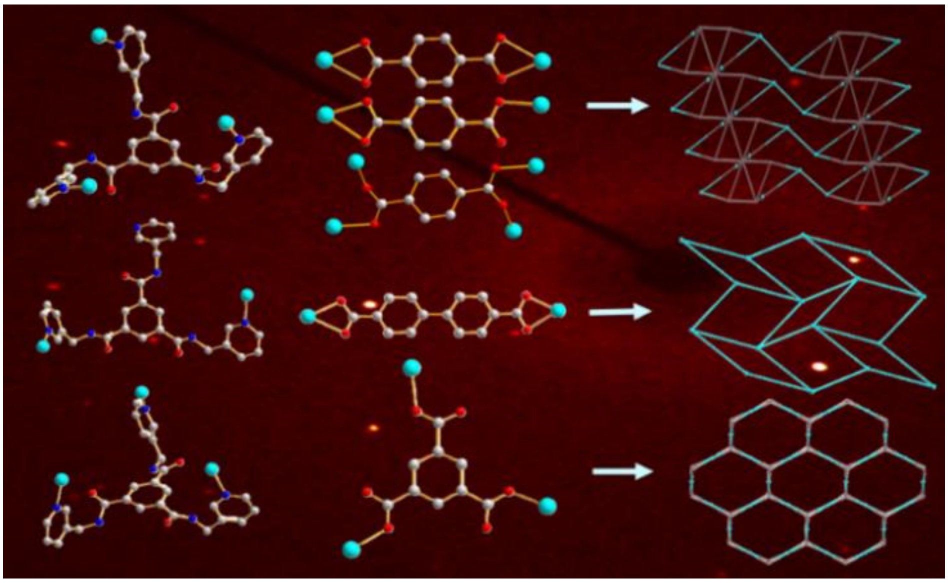
Reactions of *N,N',N''*-tris(3-methylpyridyl)trimesic amide (**L**) and $Cd(OAc)_2 \cdot 2H_2O$ with various polycarboxylic acids afforded $\{[Cd_2(\mathbf{L})(1,4\text{-BDC})_2(H_2O)_2] \cdot 2H_2O\}_n$ (1,4-H_2BDC = benzene-1,4-dicarboxylic acid), **1**, $\{[Cd(\mathbf{L})(4,4'\text{-BDC})(H_2O)] \cdot H_2O)\}_n$ (4,4'-H_2BDC = biphenyl-4,4'-dicarboxylic acid), **2**, and $\{[Cd_3(\mathbf{L})_2(1,3,5\text{-BTC})_2(H_2O)_6] \cdot 15H_2O\}_n$ (1,3,5-H_3BTC = benzene-1,3,5-tricarboxylic acid), **3**, which have been structurally determined by using single-crystal X-ray diffraction. Complexes **1–3** display 2D layers with $(3 \cdot 8^2)_2(3^2 \cdot 4)_2(3^6 \cdot 4^4 \cdot 5^2 \cdot 8^4 \cdot 9^6 \cdot 10^5 \cdot 11)$, $(4^4 \cdot 6^2)$-**sql** and $(4^2 \cdot 12^4)_3(4^3)_4$-3,4L129 topologies, respectively, indicating that the identities of the polycarboxylate ligands involving length and shape play important roles in determining the structural diversity. Complexes **1** and **2** show stabilities in various solvents and display high selectivity toward sensing of Fe^{3+} ions with low detection limits and good reusability up to five cycles.

Keywords: coordination polymer; polycarboxylic acid; sensing properties



Inorganic Chemistry (IC-P-004)

Designed synthesis of Co(II) coordination polymers for evaluation of structural transformations

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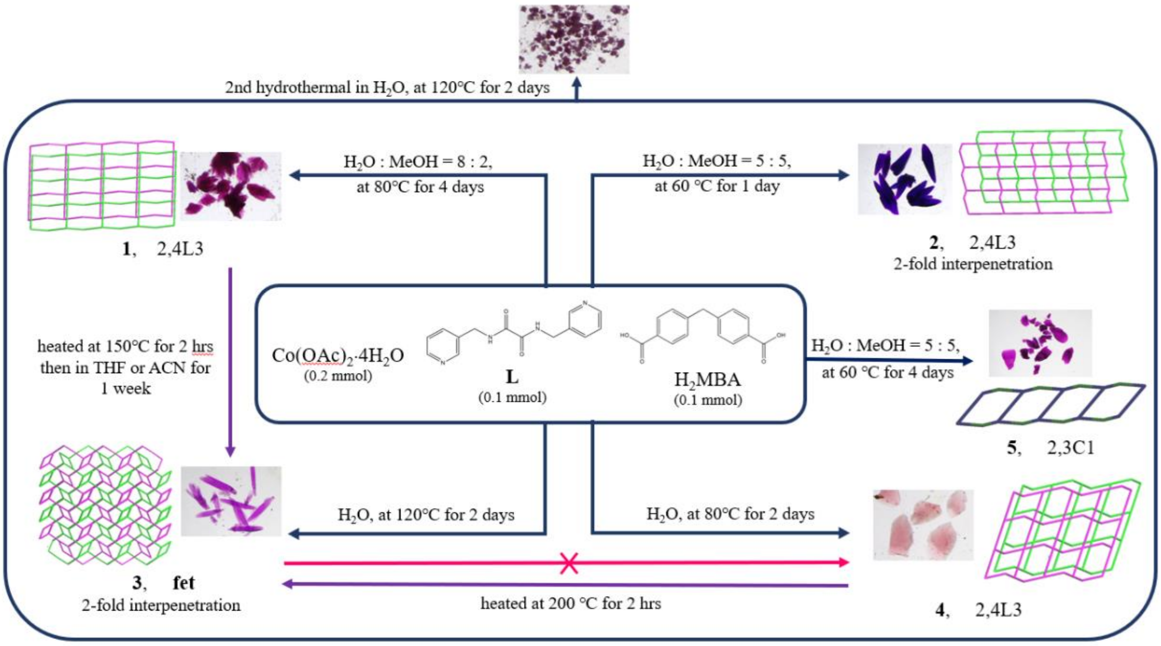
Five coordination polymers constructed from Co(II) salts, *N,N'*-bis(3-pyridylmethyl)oxalamide (**L**) and 4,4'-methylenedibenzoic acid ($\mathrm{H_2MBA}$), $\{[\mathrm{Co}(\mathbf{L})(\mathrm{MBA})(\mathrm{H_2O})]\cdot\mathrm{H_2O}\}_n$, **1**, $\{[\mathrm{Co}(\mathbf{L})(\mathrm{MBA})]\cdot 4\mathrm{H_2O}\}_n$, **2**, $\{[\mathrm{Co}(\mathbf{L})(\mathrm{MBA})]\cdot 0.25\mathrm{H_2O}\}_n$, **3**, $[\mathrm{Co}(\mathbf{L})(\mathrm{MBA})(\mathrm{H_2O})_2]_n$, **4**, $\{[\mathrm{Co}(\mathbf{L})0.5(\mathrm{MBA})(\mathrm{H_2O})_2]\cdot\mathrm{CH_3OH}\}_n$, **5**, are reported, which have been structurally characterized by using single crystal X-ray crystallography. Complexes **1** and **4** have the same formula, but differ in the number of coordinated and cocrystallized water molecules, whereas **2** and **3** form a pair of supramolecular isomers with different numbers of cocrystallized water molecules. Complexes **1** and **4** show interdigitated 2D layers with the $(6^4\cdot 8\cdot 10)(6)$-2,4L3 topology, which differ in the ligand conformations of **L** and bonding modes of MBA^{2-}. Complex **2** shows 2-fold interpenetrated 2D layers with the $(6^4\cdot 8\cdot 10)(6)$-2,4L3 topology and **3** displays a 2-fold interpenetrated 3D framework with the $(4\cdot 6^2)(4\cdot 6^6\cdot 8^3)$-**fet** topology, whereas **5** is a 1D ladder with the $(6^2\cdot 10)(6)$-2,3C1 topology, indicating that the coordination and/or cocrystallization of solvent molecules are important in determining their structural diversity. The structural transformations of **1–4** are also evaluated.

Keywords: coordination polymer; structural transformation; topology; interpenetration



Inorganic Chemistry (IC-P-012)

Base catalytic properties of Lindqvist-type polyoxotantaletes

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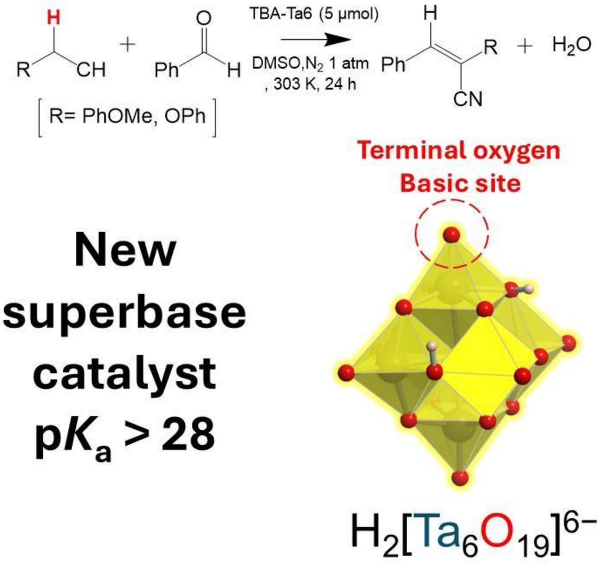
Polyoxomethalates have been extensively studied as intriguing catalysts [*Chem. Rev.* **2015**, *115*, 4893–4962]. Recently, we have reported that Lindqvist-type $[Nb_6O_{19}]^{8-}$ associated with tetrabutylammonium (TBA) cations (**TBA-Nb6**) was superbase catalysts for Knoevenagel condensation (KC) reactions of active methylene substrates with $pK_a > 26$, exhibiting proton abstraction from base indicators with pK_a up to 26.5 [*Angew. Chem. Int. Ed.* **2024**, *63*, e202401526]. From density function theory (DFT) calculations, Lindqvist-type $[Ta_6O_{19}]^{8-}$ (**Ta6**) is expected to show a higher negative natural bonding charge than **Nb6**, suggesting the stronger base catalytic properties of **Ta6** [*J. Phys. Chem. C* **2018**, *122*, 29398−29404]. In this study, we synthesized **TBA-Ta6** using microwave-assisted hydrothermal method, characterized it as $TBA_6H_2[Ta_6O_{19}]$ by ESI-MS and elemental analysis, and investigated its base catalytic properties. From Hammett indicator titration results, **TBA-Ta6** was found to have basic sites for proton abstraction with pK_a up to 26.5 like **TBA-Nb6**. As for catalytic properties, **TBA-Ta6** served as a homogeneous catalyst for KC reactions of benzaldehyde with 4-methoxyphenylacetonitrile ($pK_a = 23.8$) and phenoxyacetonitrile ($pK_a = 28.1$). **TBA-Ta6** showed higher product yield in the KC reaction of phenoxyacetonitrile with $pK_a = 28.1$ than **TBA-Nb6**, suggesting the stronger base catalytic properties of **TBA-Ta6**.

Keywords: polyoxotantaletes; base catalyst; Hammett indicator titration; Knoevenagel condensation reaction



Inorganic Chemistry (IC-P-013)

Ortho-carborane appended multi-resonance TADF emitters for high-efficiency blue OLEDs

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Ortho-carborane (1,2-*closo*-$C_2B_{10}H_{12}$), an electron-deficient icosahedral boron cluster, has received considerable attention as a steric and electronic building block for constructing various luminophores over the past decade due to its steric bulkiness and three-dimensional electron delocalization through three-center, two-electron bonds. The emissive excited state of the *o*-carboranyl luminophores can be accessed through the locally excited (LE) or intramolecular charge transfer (ICT) states, depending on the degree of cage rotation. Since the electronic effects of *o*-carborane can also vary depending on the π-systems used, the choice of the parent π-luminophore becomes a critical factor in tuning the excited-state properties. To understand the role of *o*-carborane in controlling the photophysical properties of various luminophores, we employed a multi-resonance induced thermally activated delayed fluorescence (MR-TADF) core as a new luminophoric π-skeleton to create novel *o*-carboranyl TADF emitters. We have prepared *o*-carboranyl luminophores in which *o*-carborane moieties are incorporated at the periphery of the B,N-doped MR-TADF core. It was shown that the inherent local emission characteristics of the MR-emitting core are retained but tuned through *o*-carborane substitution. Our recent results on the photophysical and electroluminescent properties of *o*-carborane decorated MR-TADF emitters will be presented.

Keywords: *ortho*-carborane; multi-resonance; TADF; blue emission; OLEDs

Inorganic Chemistry (IC-P-015)

Synthesis and characterization of Ag/TiO_2/MCM-41 composite from rice husk ash

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This research presents a method for synthesizing Ag/TiO_2/MCM-41 composites using rice husk ash (RHA) as a sustainable and low-cost silica source. The objective of this study was to develop an environmentally friendly material for the adsorption and degradation of organic pollutants. RHA was converted into a high-quality silica precursor through simple acid-leaching and calcination. The resulting silica was then used to synthesize MCM-41, a mesoporous material with well-defined pore structure. Silver ions were subsequently incorporated into TiO_2 to form the Ag/TiO_2/MCM-41 composites which were characterized using various techniques, including XRD, FTIR and SEM. The results confirmed the successful formation of Ag/TiO_2/MCM-41. This study demonstrates the potential of RHA as a valuable resource for synthesizing Ag/TiO_2/MCM-41 composite. The proposed method offers a sustainable and environmentally friendly alternative to traditional silica sources, contributing to a circular economy and reducing the environmental impact of material production.

Keywords: rice husk ash; Ag nanoparticles; TiO_2; MCM-4

Inorganic Chemistry (IC-P-018)

Molecular tuning of copper catalysts for selective CO_2 fixation and electrocatalytic conversion

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The efficient capture and conversion of CO_2 into valuable products is a pivotal strategy for addressing climate change and mitigating CO_2 emissions. This study builds upon previous investigations of Holm's Cu(II) complexes with pyridine-2,6-dicarboxamide scaffolds, aiming to exploit their biomimetic property of CO_2 fixation and explore potentially electrocatalytic CO_2 reduction. However, the inherent instability of these complexes compromises their catalytic performance.

To overcome this limitation, we designed a redox-active ligand incorporating thioether moieties, hypothesizing that the inclusion of soft sulfur donors would stabilize the Cu(I) oxidation state and prevent catalyst degradation. We synthesized and evaluated two distinct complexes: a macrocyclic thioether complex and a non-macrocyclic thioether complex, assessing their stability and catalytic efficacy. The macrocyclic thioether complex demonstrated exceptional electrochemical CO_2 reduction activity, selectively converting CO_2 to CO with a Faradaic efficiency of approximately 85%.

To elucidate the reaction mechanism and catalytic pathway of these complexes, we employed a suite of spectroscopic and electrochemical techniques, including EPR, IR, UV-Vis, and cyclic voltammetry. These mechanistic results provide critical insights into the design principles governing the stability and efficiency of CO_2 reduction catalysts, offering a pathway toward more robust and effective electrocatalysts for carbon capture and utilization.

Keywords: green chemistry; copper complex; CO_2 reduction; electrocatalysis

Inorganic Chemistry (IC-P-022)

Lanthanide coordination chemistry and its coupling with mobile phone camera for use as recyclable sensing probe of trace-water in organic solvents

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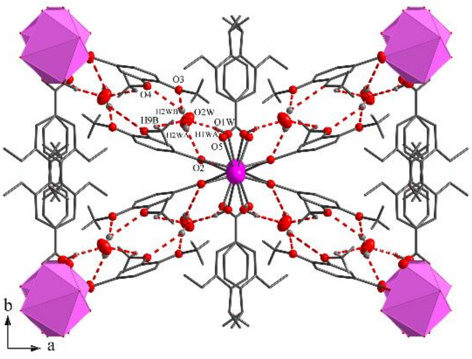
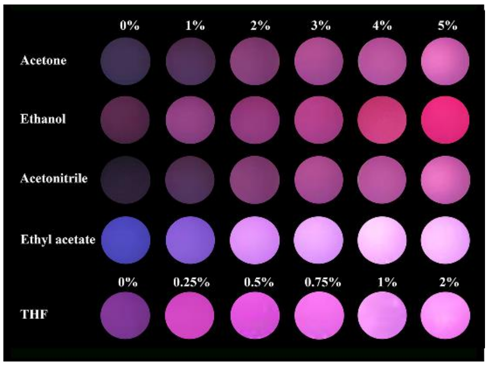
A series of ten new lanthanide coordination polymers, *i.e.* $[Ln^{III}(dmba)_3(H_2O)_2]\cdot 2H_2O$, where Ln^{III} = La^{III} (**I**), Pr^{III} (**II**), Nd^{III} (**III**), Sm^{III} (**IV**), Eu^{III} (**V**), Gd^{III} (**VI**), Tb^{III} (**VII**), Dy^{III} (**VIII**), Ho^{III} (**IX**) and Er^{III} (**X**), were synthesized and characterized. Founded on the flexible coordination chemistry and extreme oxophilicity of the trivalent lanthanides (Ln^{III}), their photoluminescent properties were studied from which the dependence on the dehydration/rehydration has been disclosed. Based on the turn-off (dehydration) and turn-on (rehydration) of the red emission of Eu^{III}, a mobile phone camera and freeware application, the use of **V** in the colorimetric sensing of trace water in polar organic solvents has been innovated. With respect to ethanol, acetonitrile, and acetone, linear correlations can be established from which the excellent limits of detection and quantification as well as its recyclability have been achieved. The underlying mechanism is postulated.

Keywords: lanthanide; coordination polymer; photoluminescence; colorimetric sensing; water sensing





Inorganic Chemistry (IC-P-024)

Selective detection of divalent cations (Cu^{2+}, Zn^{2+}, Pb^{2+}) and anions (SO_4^{2-}, S^{2-}, CO_3^{2-}) using a pH-sensitive multi-functional schiff base in neutral medium

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A novel Schiff base-based probe (L) has been synthesized and characterized using HR-MS, FT-IR, and both ^1H and ^{13}C NMR spectroscopy. The Schiff base framework offers selective binding sites for multiple cations and anions, producing distinct optical responses. Upon interaction with cations such as Cu^{2+}, Zn^{2+}, and Pb^{2+}, and anions like CO_3^{2-}, S^{2-}, and SO_4^{2-}, the probe undergoes a visible color change from pale yellow to various yellow hues. This change is attributed to metal complex formation (e.g., M_3L_2) and ligand deprotonation in the presence of anions. Notably, complexes with Zn^{2+} and S^{2-}/ CO_3^{2-} exhibit fluorescence, facilitating the detection of Cu^{2+} and SO_4^{2-} with detection limits of 8.48 µM and 10.47 µM, respectively, via Stern–Volmer analysis. Alkaline conditions (pH > 8) enhance fluorescence due to deprotonation of phenolic –OH and amide –NH groups. Cu^{2+} ions quench this emission, which is restored upon chelation with EDTA. This reversible fluorescence response supports the construction of a molecular logic gate illustrating a TURN-OFF-TURN-ON mechanism. Overall, probe L demonstrates excellent multifunctional sensing capabilities for practical analytical applications.

Keywords: selective binding, fluorescent probe, analyte sensing, logic gate

Inorganic Chemistry (IC-P-025)

Tailored rhenium tricarbonyl complexes incorporating 2,6-bis(pyrazol-1-yl)pyridine ligands for efficient electrochemical carbon dioxide reduction

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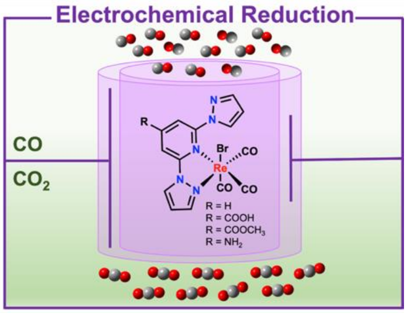
Rhenium(I) tricarbonyl complexes incorporating 2,6-bis(pyrazol-1-yl)pyridine (bpp) ligands with electron-withdrawing (-COOH and -$COOCH_3$) and electron-donating (-NH_2) groups were synthesized to study the effect of ligand electronics on electrocatalytic CO_2 reduction. Each complex adopts a bidentate coordination mode, leaving one pyrazolyl arm unbound and freely rotating, a feature proposed to promote proton-coupled electron transfer (PCET). Cyclic voltammetry under CO_2-saturated conditions with acetic acid revealed that ligand substitution strongly modulates catalytic behavior. The **Re-bppCOOH** complex, bearing a strongly electron-withdrawing group, exhibited the highest activity (-176.9 μA at -2.72 V), attributed to the stabilization of reduced intermediates and improved PCET efficiency. In contrast, **Re-bppCOOCH$_3$** showed moderate activity, while the electron-donating **Re-bppNH$_2$** complex displayed reduced currents (-164.1 μA at -2.69 V), consistent with destabilization of catalytic species. The substituted **Re-bpp** complex demonstrated intermediate performance (-106.0 μA at 2.66 V). These results showed the electronic and steric properties of the bpp ligand, particularly the role of the non-coordinating pyrazolyl unit, govern catalytic efficiency. This work provides mechanistic insight into ligand-assisted CO_2 reduction and offers design principles for developing more efficient molecular electrocatalysts.

Keywords: electrocatalysis; CO_2 reduction; rhenium complexes; ligand effects; proton-coupled electron transfer (PCET)



Materials Science and Nanotechnology (MN-P-003)

Synthesis and characterization of UV-light-driven Pd nanoparticles/$ZnWO_4$ nanorods photocatalyst by photoreduction deposition method

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UV-light-driven Pd nanoparticles/$ZnWO_4$ nanorods photocatalyst was prepared by photoreduction deposition method. Effects of phase, morphology, atomic vibration and surface area on different weight contents of Pd loaded on $ZnWO_4$ nanorods were analyzed by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, BET surface area analysis, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS) instruments and discussed in this research. They showed that the metallic Pd nanoparticles were uniformly decorated on the high crystalline wolframite $ZnWO_4$ nanorods. The effect of weight of Pd loading on the surface of one-dimensional $ZnWO_4$ nanorods on photocatalytic degradation of rhodamine B (RhB) under UV light irradiation has been studied and discussed in this research. The 5% Pd/$ZnWO_4$ nanocomposites exhibited the highest RhB degradation of 92.89% within 240 min under UV light irradiation because of the Pd nanoparticles played the role in surface plasmon resonance (SPR) effect to produce more photo-induced charge pairs and extend the lifetime of photo-induced charge pairs of the composites.

Keywords: Pd−$ZnWO_4$ interfaces; photoreduction synthesis; photocatalysis

Materials Science and Nanotechnology (MN-P-009)

Enhanced photothermal water evaporation and energy generation using copper nanoparticle-decorated carbon/PDMS nanocomposites

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This work presents a facile hydrothermal approach for synthesizing a novel Cu-nanoparticle (Cu-NP) decorated hydrothermal carbonaceous carbon (Cu-HTCC) hybrid material. Glucose acts as a dual-functional agent, simultaneously reducing Cu^{2+} ions to Cu NPs and serving as a carbon precursor. The resulting Cu-HTCC exhibits significantly enhanced visible-near-infrared light absorption, attributed to the synergistic effect of localized surface plasmon resonance (LSPR) from Cu NPs and the unique electronic structure of the HTCC matrix. Flexible 2D and 3D Cu-HTCC/PDMS (polydimethylsiloxane) nanocomposites were fabricated, demonstrating excellent solar light absorption and promising performance in both photothermal water evaporation (up to 1.47 kg m^{-2} h^{-1}) and thermoelectric power generation (up to 32.1 mV) under 1 sun illumination. This multifunctional hybrid material offers a compelling platform for sustainable solar energy harvesting and water management applications. [*Small* **2024**, *20*, 2403565]

Keywords: interfacial water evaporation; localized π systems; metal–semiconductor hybrids; plasmonics; thermoelectric power generation

Nickel-based materials for applications on supercapacitor

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Increasing environmental concerns about fossil fuels have led to research on alternative energy storage solutions [*Energy Strategy Rev.* **2024**, *54*, 101482]. Among these, supercapacitors stand out due to their long cycle life and high specific capacitance [*Fuel.* **2023**, *337*, 127125]. Electrode material selection is crucial for supercapacitor performance. Carbon-based materials, conductive polymers, and metal oxides are widely used in literature. While ruthenium oxide offers high specific capacitance, its high cost and scarcity limit its use [*Int. J. Hydrogen Energy.* **2024**, *70*, 10–28]. Nickel oxide and hydroxide are promising alternatives due to their high capacitance, low cost, and tunable nanostructures. However, challenges such as low electrical conductivity and volume expansion necessitate optimized composite production methods [*Crit. Rev. Solid State Mater. Sci.* **2021**, *46*, 553–586]. In this study, nanoflower-shaped nickel oxide and hydroxide were synthesized using the co-precipitation method and employed as electrode materials in supercapacitors. Structural characterization techniques, including XRD, SEM and XPS, were used to confirm the properties of the nickel oxide/hydroxide powders. Subsequently, supercapacitors incorporating these powders were electrochemically characterized. Nanoflower-shaped nickel oxide exhibited high capacitance retention and excellent specific capacitance, making it a promising candidate for supercapacitor applications.

Keywords: nickel oxide hydroxide; electrode; supercapacitor; co-precipitation

Materials Science and Nanotechnology (MN-P-013)

Elimination of THP by separation of extracellular vesicles from urine samples

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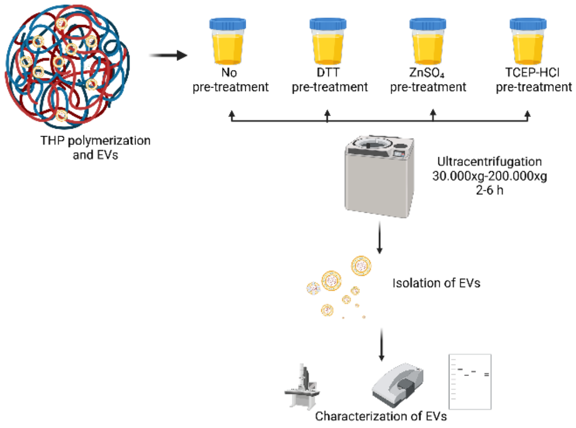
The most significant challenge in the isolation of extracellular vesicles (EVs) from urine is the presence of Tamm–Horsfall protein (THP) in high concentrations. THP, a cysteine-rich protein, exists in urine as a high molecular weight polymer that assembles into filaments. In the present study, a range of methodological approaches were employed to inhibit the polymerization of disulfide bonds with THP using DTT, $ZnSO_4$, TCEP-HCl, and the efficiency of these approaches in EV isolation from urine was evaluated. The isolation process of human urine EVs involved ultracentrifugation steps (30,000-200,000xg at 2-6h) following incubation with DTT, $ZnSO_4$, and TCEP-HCl. The isolated EVs were characterized using TEM, zeta sizer and CD63 protein. The study revealed that while $ZnSO_4$ and TCEP-HCl can be utilized at low temperatures, ambient temperature is a crucial factor for the efficacy of DTT. The isolation process proved to be effective within a time frame of 10-30 minutes in the presence of DTT and TCEP-HCl. While the isolation of EVs (size:10–300 nm) with DTT, $ZnSO_4$, and TCEP-HCl is indeed effective in proteomic studies. This is due to their interaction with the cysteines present in the structure of EVs, affecting both the pure particle number and the morphology. (Funding: This study was supported by a grant TUBITAK- 124S213 and TUBA-GEBIP)

Keywords: extracellular vesicles; THP; cysteine-rich protein; urine exosomes



Materials Science and Nanotechnology (MN-P-014)

Development of aptamer-linked nanoparticles for cervical cancer diagnosis

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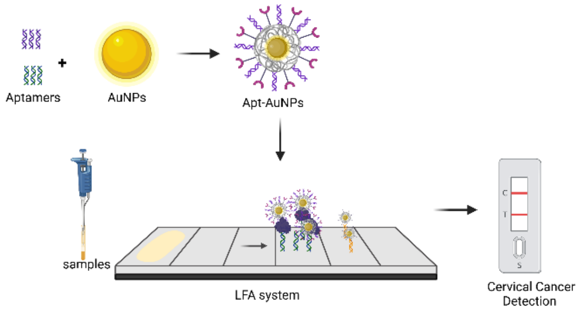
Aptamers (Apt) are short, single-stranded DNA or RNA molecules that can recognize target molecules based on their specific three-dimensional folding. They are superior to antibodies in terms of low cost and short production time, thermal stability, very low/no immune response and lyophilizability. The use of aptamers instead of antibodies in LFA systems is rapidly increasing. In this study, aptamers targeting specific proteins in cervical cancer were used and gold nanoparticles (AuNPs) were developed. Apt-AuNPs were characterized by FTIR and SEM analysis. Specificity tests of aptamers against HPV proteins were performed and Apt-AuNPs were tested by dot blot using Hela cancer cells. It was shown that the color intensity changed in samples at different concentrations and the sensitivity of AuNPs changed depending on the aptamer binding capacity. When the stabilization of aptamers in binding buffers was tested, it was shown that they were resistant to pH changes, but DNAse-RNAse conditions needed to be stabilized. As a result, the developed LFA system can discriminate positive and negative cervical cancer patients from urine samples, and its sensitivity varies depending on the size of Apt-AuNPs. Therefore, the use of AuNPs with aptamers in LFA systems is fast and low cost for cervical cancer detection. (Funding: This study was supported by a grant TUBITAK-223S614 and TUBA-GEBIP)

Keywords: aptamer; cervical cancer; lateral flow; diagnosis



Materials Science and Nanotechnology (MN-P-021)

Synthesis and characterization of sol-gel bioactive glass standards for *in vitro* apatite formation

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Bioactive glasses are widely recognized for their ability to form hydroxyapatite (HA) in physiological environments, a key factor in bone regeneration. Standardizing bioactive glass materials is essential for evaluating apatite-forming ability, particularly in simulated body fluid (SBF) studies. However, most existing standards are based on melt-quench-derived glasses, which may exhibit different bioactivity and textural properties compared to sol-gel-derived materials. This study proposes a novel fabrication method for sol-gel-derived glass standards and compares their apatite-forming ability with melt-quench-derived glass standards following ISO/FDIS 23317. Sol-gel-derived bioactive glass powders were synthesized with optimized processing parameters and characterized using X-ray fluorescence (XRF) for composition, X-ray diffraction (XRD) for phase identification, and scanning electron microscopy (SEM) for morphology. Ion release in SBF was analyzed to assess degradation, while hydroxyapatite formation was evaluated using XRD and SEM after immersion in SBF. Results showed that sol-gel-derived glass standards exhibited well-defined particle size distribution, controlled degradation, and enhanced HA nucleation compared to melt-quench-derived glass. These findings suggest that sol-gel-derived standards provide a valuable alternative for assessing the in vitro bioactivity of bioactive glasses in bone tissue engineering applications.

Keywords: bioactive glass; sol-gel; hydroxyapatite; *in vitro* bioactivity; ISO/FDIS 23317

Materials Science and Nanotechnology (MN-P-022)

Chirality enhancement in polymer films for CPL generation and its application to microalgae cultivation

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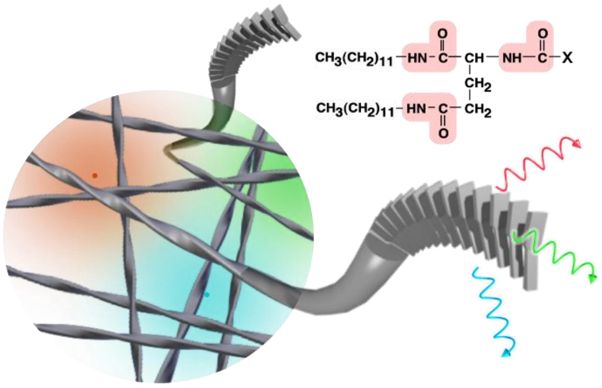
Circularly polarized light (CPL), which has unique characteristics not found in linear light, is expected to be used in a variety of applications as a next-generation light source such as biometric authentication, medical sensing, and high-density memory. On the other hand, many living materials universally have chiral structures such as chiral carbon and helical structures, but CPL has not been utilized in applied research because of its lack of practicality in terms of optical purity. Therefore, we focused on the phenomenon that the glutamide derivative developed by us forms a chiral supramolecular assembly in a solution system, and when it is doped with a fluorescent dye, secondary chirality is induced in the dye, resulting in high-purity circularly polarized luminescence. Based on this finding, we aimed to induce amplified chirality in a polymer, and to apply the generated CPL to the cultivation of microalgae. For this purpose, we mixed the supramolecular system consisting of a fluorescent dye and glutamide lipids in a transparent polymer such as PMMA, and prepared a polymer film that generates CPL. In this report, we also consider the effect of CPL on photosynthesis through research into cultivating microalgae by irradiating seawater with left- and right-handed CPL.

Keywords: self-assembly; induced secondary chirality; circularly polarized luminescence



Glutamide-derivatives assemble chirally into nanofibers in polymers to produce highly pure CPL

Enhancing mechanical properties of biodegradable plastic films reinforced with crystal nanocellulose for sustainable packaging

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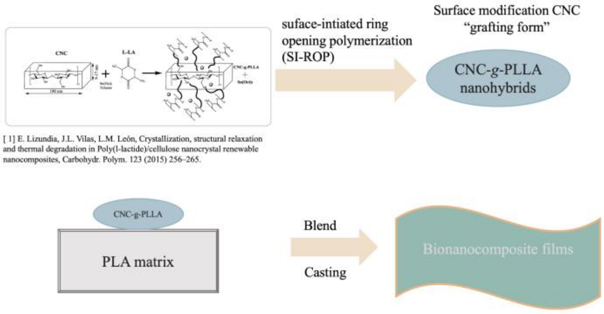
Amid growing environmental concerns, bio-based polymers and advanced processing technologies are gaining interest as sustainable alternatives to fossil fuel-derived materials. In packaging applications, petroleum-based plastics are being replaced with bio-nanocomposites, which offer lightweight, high-performance, and eco-friendly solutions. Biopolymers such as starch, cellulose derivatives, PLA, PCL, PBS, and PHB exhibit mechanical strength, barrier functionality, and biodegradability, making them ideal for sustainable packaging.

Previously, cellulose nanocrystals (CNCs) were synthesized from microcrystalline cellulose (MCC) via sulfuric acid hydrolysis at 34% w/w (CNC1) and 64% w/w (CNC2). TEM and SEM analyses confirmed that CNC2 had smaller dimensions. PLA/CNC1 and PLA/CNC2 bionanocomposite films were then prepared at 1 wt.% and 3 wt.%, with FTIR and SEM confirming their structural integrity. Higher CNC concentrations resulted in increased surface roughness and self-aggregation.

This study aims to improve PLA/CNC film homogeneity by modifying CNCs via surface-initiated ring-opening polymerization (SI-ROP) of L-lactide, forming CNC-g-PLLA nanohybrids (20/80, 10/90, 5/95). These were incorporated into PLA at 1 wt.% and 3 wt.% and evaluated for thermal, mechanical, and morphological properties. This research advances sustainable packaging materials, reducing single-use plastic waste and environmental pollution.

Keywords: biodegradable plastic; nanocomposite; polylactic acid; crystal nanocellulose



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Materials Science and Nanotechnology (MN-P-025)

Mortar for masonry from recycled concrete and mortar aggregates

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This study addresses the issue of construction waste and excessive consumption of natural resources in the construction industry. The concept of “Green Concrete” was introduced to mitigate environmental impacts. This research aims to develop and formulate a mortar for masonry using recycled concrete and mortar aggregates (Recycle Concrete Aggregate, RCA) as a complete replacement (100%) for natural sand and gravel. The feasibility of RCA utilization was examined to ensure compliance with the Industrial Product Standard for masonry mortar (TIS 598-2560). The developed mortar formulations were evaluated based on their physical and mechanical properties, including bond strength, water retention, compressive strength, and setting time. The results indicate that RCA-based mortar formulations meet all industrial standard requirements and can be commercially produced. This research demonstrates that using recycled concrete and mortar aggregates can reduce construction waste by up to 80% while enhancing the value of waste materials. Additionally, it contributes to the reduction of natural resource consumption, minimizes environmental impact, and supports sustainable development in the construction industry.

Keywords: recycle concrete aggregate; waste concrete; green concrete; masonry mortar

Materials Science and Nanotechnology (MN-P-027)

Discovery of novel fluorescence gold nanoclusters for bio-imaging applications

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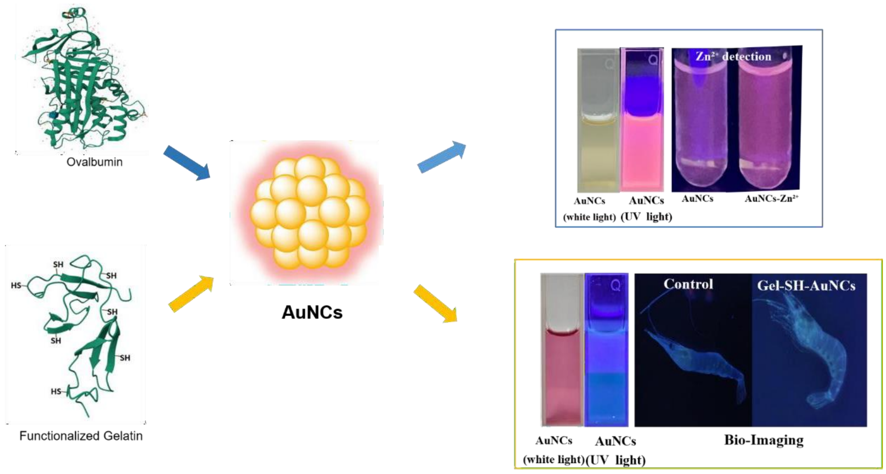
Gold Nanoclusters (AuNCs) are nanomaterials consisting of multiple gold atoms with a size < 2 nanometer. AuNCs have high surface area and exhibit fluoresce nce emission in the near infrared (NIR) region with the range of 800–2500 nanometer, suitable applicable for bio-imaging research. According to its high stability characteristic, AuNCs can be applied in various fields, for example sensor development, metal detection, and bio-imaging applications. Therefore, this research focuses on synthesizing gold nanoclusters from various proteins, such as ovalbumin and functionalized gelatin. Additionally, we examined the stability of the synthesized gold nanoclusters by using pH study, the solvent effect and the sensing performance towards metal ions, showing the great specific with Zn^{2+}. Besides, we investigated the chemical integrity and optical properties using UV-Visible and Fluorescence spectroscopy, Transmission Electron Microscopy (TEM), and X-ray Photoelectron Spectroscopy (XPS) techniques. Finally, bio-imaging applications were performed by using shrimp models.

Keywords: gold nanoclusters; bio-imaging; fluorescence



Hierarchical cotton-based membranes for versatile water remediation

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The simultaneous separation of oil/water mixtures and catalytic degradation of organic pollutants remains a critical challenge in sustainable wastewater treatment. This study introduces a hierarchically structured cotton-based membrane fabricated through sequential deposition of polydopamine (PD), Au nanocatalysts, and iron oxide nanoneedles. The PD layer serves as a templating matrix for precise nanocatalyst immobilization, while the vertically aligned iron oxide nanoneedles enhance solvent diffusion via capillary effects. This membrane exhibits dual functionality: efficient separation of large volumes of oil/water mixtures and ultrafast catalytic reduction of toxic organic pollutants—achieving over 99% conversion of 4-nitrophenol to 4-aminophenol within 30 seconds and methylene blue to leucomethylene blue in 5 minutes. The synergy between nanocatalysts and nanostructure-enhanced mass transport enables high-performance wastewater treatment, offering significant potential for industrial-scale water remediation.

Keywords: membrane; oil/water separation; hierarchical structure; wastewater treatment; nanocatalysts

Materials Science and Nanotechnology (MN-P-030)

Rapid synthesis of manganese oxide nanocatalysts for ultrafast dye degradation

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Manganese oxide nanocatalysts (MONs) have emerged as effective oxidizers for organic pollutant removal due to their high surface area and reactivity. This study introduces a rapid, one-minute molten salt synthesis method for MONs, enabling effective catalytic degradation of various toxic organic pollutants. The MONs, with a crystalline Mn_3O_4 phase and a particle size range of 20-50 nm, were characterized using XRD, SEM, TEM, and EDX analysis. Under acidic conditions (pH = 2) and without external energy inputs such as light or heat, MONs achieved remarkable degradation efficiencies within 30 seconds: 95.59% for methyl orange (MO), 98.72% for acid orange 7 (AO7), 76.30% for Congo red (CR), 96.28% for methyl blue (MB), and 84.12% for rhodamine B (RhB). Furthermore, MONs retained an MO degradation efficiency of 94.22**%** or higher after 8 reuse cycles and demonstrated robust performance (95.12%-96.19%) under high-salinity conditions. X-ray photoelectron spectroscopy (XPS) analysis and radical scavenger tests revealed that the rapid processing capability of MONs is attributed to their exceptional redox stability and the presence of abundant surface oxygen vacancies.

Keywords: manganese oxide; nanocatalyst; wastewater treatment; dye degradation; molten slat method

Materials Science and Nanotechnology (MN-P-036)

Chiroptical properties of perovskite quantum dots prepared in chiral supramolecular gel films

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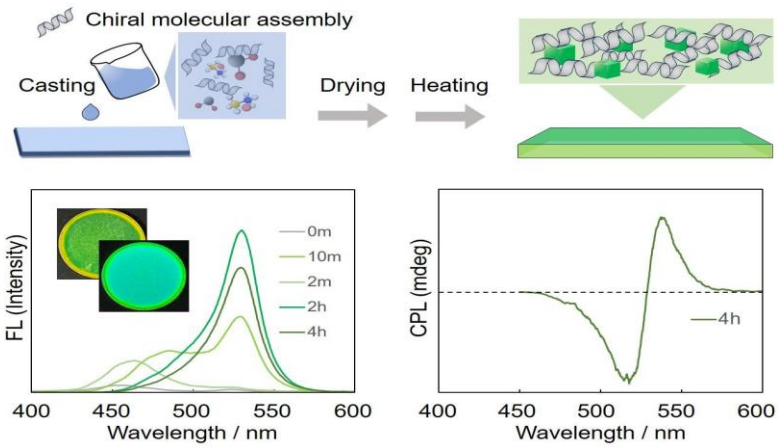
Recently, perovskite quantum dots (PQDs) exhibiting chiroptical properties have been reported for the materials in optical devices. Here, we introduce a novel approach for one-step synthesis of PQDs in the chiral supramolecular gel and discuss emission and chiroptical properties. -

PQD–chiral gelator films were prepared by casting of *N*,*N*-dimethylformamide solution of $CH_3NH_2\cdot HBr$, $PbBr_2$ and the ornithine-derived chiral gelator on a quartz plate and dried at 20 °C then heated at 100 °C. Emission peaks appeared at 460 nm in dried film before heating and red-shifted to 530 nm with intensity enhancement by heating. The fluorescence lifetime of the emission at 530 nm was 26 ns which was longer than that at 460 nm. These findings indicated that the size of PQDs increased by heating. Chiroptical properties of PQDs were evaluated with circular dichroism (CD) and circularly polarized luminescence (CPL) spectrophotometers. CD signal was observed around the absorption band (360 nm) of PQD before heating, and red-shifted to 530 nm. After heating for 4 h, bisignate CPL signals were observed at 517 nm (glum: -5.8×10^{-4}) and 540 nm (glum: 5.7×10^{-4}), which were rotation angle independent. It was speculated that the chirality of ornithine-derived self-assembly transferred to the PQDs.

Keywords: perovskite quantum dots; chirality; circular dichroism; circularly polarized luminescence; supramolecular assembly



Materials Science and Nanotechnology (MN-P-037)

Standardization of density measurement procedures for nanocarbon flakes

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Nanocarbon materials, particularly graphene and carbon nanotubes (CNTs), have attracted significant attention as functional materials across diverse applications. While standardized methods for evaluating their electrical, physical, and chemical properties have been developed, density measurement remains a challenge due to the fluffy, low-density nature of nanocarbon flakes. This challenge can be addressed by proposing a comprehensive testing strategy based on the developing IEC TS 62607-35 standard: "Graphene – Density: free pouring, tapping, compressing" method. Our methodology employs a modified commercial load tester to sequentially assess apparent density, tap density, and compressed density of nanocarbon flakes. We selected two types of nanocarbon flakes—graphene and CNTs—with varying apparent densities to evaluate compressibility as a function of applied pressure. Morphological analysis using Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) was conducted to explore the relationship between flake structure and density. Additionally, Raman spectroscopy was utilized to investigate structural integrity and volumetric recovery under specific compressibility conditions. This study can provide valuable procedures to quantify nanocarbon flake density, facilitating advancements in nanocarbon-based applications.

Keywords: density; graphene flakes; carbon nanotubes; bulk density; standardization

Materials Science and Nanotechnology (MN-P-039)

Highly conductive multifunctional iron incorporated polythiophene nanocomposite: A nanocatalyst for nitrobenzene reduction in aqueous medium and an efficient room temperature methanol gas sensor

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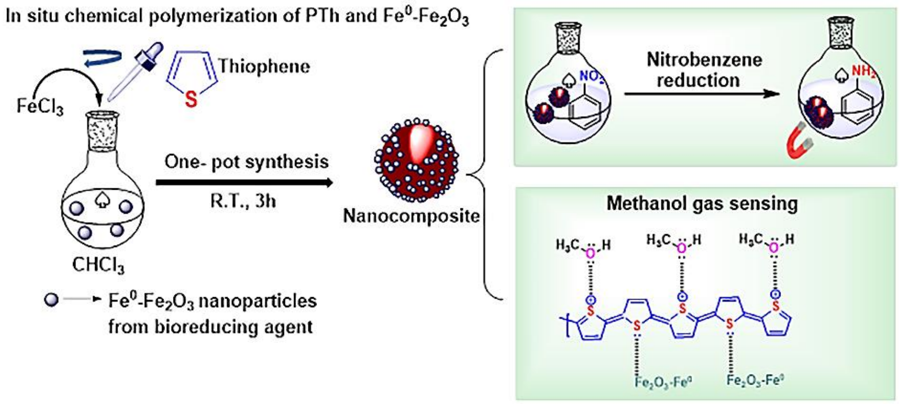
This study reports the synthesis and application of a polythiophene-iron oxide (PTh-Fe^0-Fe_2O_3) nanocomposite as a highly effective catalyst for the selective reduction of nitroaromatics in an aqueous environment. The nanocomposite was synthesized using *in-situ* chemical polymerization, with Fe^0-Fe_2O_3 nanoparticles synthesized using *Camellia sinensis* leaf extract as a reducing and stabilizing agent. Characterization techniques including XRD, FTIR, SEM-EDX, TEM, XPS, and UV-Vis spectroscopy confirmed the formation of nanocomposite. The nanocomposite demonstrated higher electrical conductivity compared to PTh alone, ranging from 20 S/cm at 313 K to 53 S/cm at 373 K. Magnetic studies indicated a saturation magnetization of 23.1 emu/g, lower than the 42.6 emu/g of Fe^0-Fe_2O_3 nanoparticles, attributed to the non-magnetic nature of PTh. The catalyst achieved a 94% yield in the reduction of nitrobenzenes under the optimum conditions [4- nitrobenzaldehyde (1 mmol), catalyst (0.04g) and water (5 mL) in air] was accomplished in 7 hours, showing broad applicability and maintaining substantial catalytic activity over six cycles. Additionally, the PTh-Fe^0-Fe_2O_3 nanocomposite exhibited notable methanol gas sensing capabilities, with sensitivity to Methanol (200 ppm), achieving sensitivity levels of 52.6, having response time of 60 seconds and recovery time of 80 seconds attributed to its n-type semiconductor behavior and diverse oxidative-reductive sites. This study is the first to introduce a novel magnetic nanocatalyst for the cost-effective and eco-friendly reduction of nitroarenes, while also demonstrating its applicability in gas sensing. [*Appl. Organomet. Chem.* **2025**, *39*, e7894]

Keywords: polythiophene; nanocomposite; gas sensor; heterogeneous catalyst; magnetic nanocatalyst



Radiation properties evaluation of holographic metasurface antennas having LC Cavity with a thickness of 200 µm

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Holographic metasurface antennas (HMAs) have the capability to swiftly and accurately beam-steering at millimeter-Wave. They allow for lightweight and compact designs, which can be used for a wide range of applications such as autonomous vehicle communication, and satellite networks compared to traditional antenna technologies. In this study, we researched HMAs in automotive radar systems to enhance future autonomous driving technology. Conventional methods utilizing multiple sensor chipsets are burdened by heightened intricacy and power usage, as well as interference between radar signals. To overcome these drawbacks, we suggest creating HMAs module using liquid-crystals (LC). Utilizing the dielectric anisotropy of LC enables precise beam-steering and conserves energy with continuous phase modulation.

In this study, LC-based HMAs were fabricated utilizing a LC with permittivity anisotropy of $\Delta\varepsilon \approx 1.1$. To achieve optimal radiation properties within the millimeter-Wave, a copper electrode with a thickness of 1 µm was created. We also designed the unit cell with a LC cell thickness of 200 µm. The completed antenna consiss of 32 unit cells. After the antenna was fabricated, its radiation properties were evaluated with varying applied voltages to ensure it was functioning correctly. The results are expected to enhance the performance of automotive radar systems.

Keywords: liquid crystal; antenna; holographic; metasurface; radar

Materials Science and Nanotechnology (MN-P-046)

$MoSe_2$-PEDOT nanocomposite for ultrasensitive electrochemical sensing of nitroaromatic compounds

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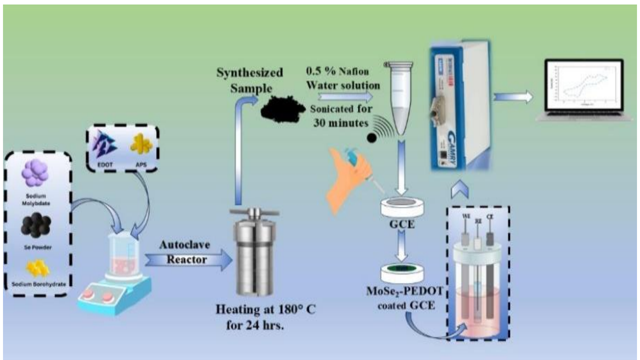
Nitroaromatic compounds (NACs) are hazardous environmental pollutants threatening human health and ecosystems due to their widespread use in industrial applications and as precursors for explosives. Developing sensitive and selective electrochemical sensors for NAC detection is crucial for environmental monitoring and security applications. Herein, we engineer a high-performance electrochemical sensor leveraging a hydrothermally synthesized $MoSe_2$-PEDOT nanocomposite for the catalytic reduction of NACs. The synergistic integration of $MoSe_2$'s rich active site, PEDOT's superior conductivity, and processable polymer matrix facilitates exceptional electrocatalytic activity toward NACs, such as nitrobenzene (NB), 2,4-dinitrotoluene (DNT), etc. The $MoSe_2$-PEDOT nanocomposite was synthesized via a facile hydrothermal method followed by in-situ polymerization, ensuring a synergistic combination, and was characterized by XRD, FESEM, and BET to confirm its structural and morphological properties. Electrochemical investigations employing cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and differential pulse voltammetry (DPV) revealed significantly enhanced electrocatalytic performance of the $MoSe_2$-PEDOT modified electrode towards the reduction of representative NACs compared to bare and single-component modified electrodes. his synergy resulted in improved peak currents and lower reduction potentials. The sensor demonstrated excellent analytical metrics, including a low limit of detection, appreciable sensitivity, good reproducibility, and satisfactory selectivity. The enhanced performance is attributed to the synergistic effect combining $MoSe_2$'s catalytic activity and PEDOT's charge transport capabilities. These findings underscore the potential of hydrothermally synthesized $MoSe_2$-PEDOT nanocomposites as effective electrode materials for developing sensitive electrochemical sensors targeting hazardous NACs.

Keywords: explosive detection; nitroaromatic compounds; electrochemical sensors; 2D-$MoSe_2$; PEDOT; electrocatalysis



Materials Science and Nanotechnology (MN-P-049)

A novel controlled release system for kasugamycin: Enhancing disease control, stability, and stress resilience in tomato crops

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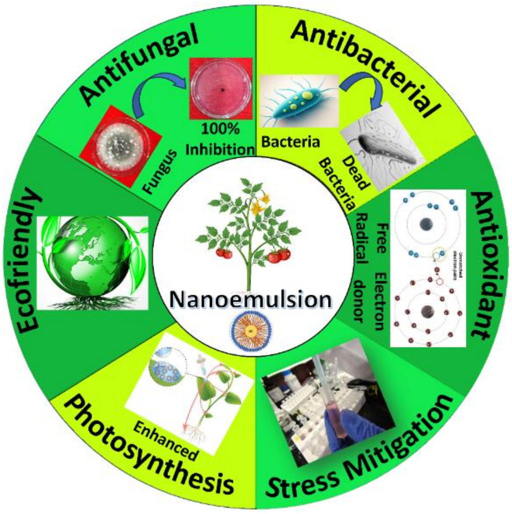
The challenges associated with traditional pesticides, such as rapid degradation due to runoff, and poor adhesion to plant surfaces, often lead to frequent reapplications and excessive use. To address these issues, our study for the first time explores kasugamycin-loaded nanoemulsion encapsulated with neem and citronella oils, designed to improve disease management and plant health in tomato crops. The nanoemulsion tested for the first time exhibited strong antibacterial activity against *Xanthomonas euvesicatoria* (bacterial leaf spot) and 100% inhibition of *Alternaria solani* (early blight) in tomato crops. It also demonstrated superior antioxidant activity, surpassing L-ascorbic acid in both DPPH and ABTS assays, highlighting its potential to mitigate oxidative stress and enhance plant resilience. DLS, TEM and zeta potential revealed the nanoemulsion small particle size and negative surface charge, enhancing bioactivity and stability. Additionally, the nanoemulsion improved spreading on tomato leaves and promoted better seed germination, root and shoot growth, and photosynthetic pigment levels showing no phytotoxic effects. It also reduced proline accumulation and lipid peroxidation, indicating effective stress mitigation and prolonged bioefficacy against pathogens. Overall, the kasugamycin-loaded nanoemulsion offers a promising, sustainable alternative to conventional pesticide formulations, providing superior and prolonged disease control, stress mitigation, and improved plant health in tomato crops.

Keywords: stress mitigation; sustainability; ecofriendly; enhanced photosynthesis; enhanced bio efficacy



Materials Science and Nanotechnology (MN-P-050)

A novel pectin-based halosulfuron-methyl nanoformulation with enhanced bio-efficacy for *Cyperus rotundus* control

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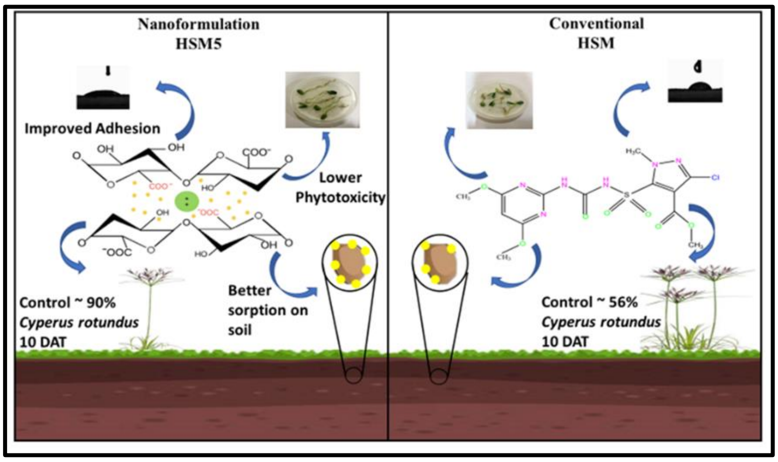
Conventional herbicide formulations often face significant challenges, including poor adhesion, inadequate spreading on plant surfaces, and leaching into the soil, reducing their effectiveness and contributing to environmental contamination. Additionally, their reliance on toxic solvents due to limited water solubility poses risks to non-target crops and ecosystems. This study aims to develop an organic solvent-free, novel pectin-based nanoformulation of halosulfuron-methyl (HSM). The herbicidal efficacy, soil adsorption behaviour, release kinetics, wettability, phytotoxicity, and impacts on non-target crop physiological parameters were examined. The pectin-based nanoherbicide (62 nm) exhibited high colloidal stability (zeta potential -35.8 mV) and achieved ~90% control of *Cyperus rotundus* within 10 days, surpassing conventional formulation (56% control), with no observed phytotoxicity in *Zea mays*. The nanoformulation demonstrated enhanced wettability characterised by a reduced contact angle and better physiological parameters in soybeans compared to the conventional formulation analysed via the petri-plate assay. Furthermore, the encapsulated HSM followed a pseudo-second-order model for sorption on sandy loam soil, suggesting improved soil retention and reduced leaching potential. The release of herbicide from pectin nanocarriers was evaluated at pH 7, and the mechanism of release of herbicide was found to follow non-Fickian behaviour, i.e. anomalous transport governed by diffusion and relaxation of the pectin chains. These findings highlight the potential of pectin-based nanoformulations as a sustainable approach for efficient and non-toxic herbicide delivery.

Keywords: nanoformulations; weed management; sustainable agriculture; pectin bio-polymer; nano-herbicide



Optimization of inulinase production from *Bacillus* sp. in yacon (*Smallanthus sonchifolius*) and in sugarcane (*Saccharum officinarum*) bagasse using response surface methodology

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Inulinase (EC 3.2.1.7) production from bacterial cultures is recommended due to their rapid fermentation with selected substrates, which can be optimized to achieve maximum enzyme production. This study focused on optimizing the extracellular production of inulinase from *Bacillus* sp. using yacon (*Smallanthus sonchifolius*) under submerged fermentation and sugarcane (*Sacharum officinarum*) bagasse under solid-state fermentation, applying response surface methodology. Box-Behnken designs were generated using Design-Expert v13 to evaluate the effects of fermentation time, media's initial substrate concentration, substrate's initial moisture content, and initial media pH on the inulinase production. The proposed model for each substrate was quadratic due to its significant result on analysis of variance (ANOVA) and the insignificant result of the lack-of-fit test. Optimal conditions for the enhanced inulinase production were 23.7 hours of fermentation time, 2.3% yacon concentration, and initial media pH of 7.4 for fermentation of yacon with inulinase activity of 8.7 U/mL; and 26.6 hours for fermentation time, 52.0% initial moisture content of sugarcane bagasse, and initial media pH of 7.0 for fermentation of sugarcane bagasse with inulinase activity of 25.0 U/gds. Experimental verifications of the models generated errors of less than 10% relative to the substrates implying that models are excellent predictors of inulinase production.

Keywords: *Bacillus* sp.; inulinase; response surface methodology; sugarcane bagasse; yacon

Natural Products, Biological Chemistry and Chemical Biology (NB-P-002)

Isolation, partial purification, and biochemical characterization of inulinase from *Bacillus* sp. produced through submerged fermentation of yacon (*Smallanthus sonchifolius*)

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Inulinase (EC 3.2.1.7) belongs to a class of enzymes that cleave the β-2,1 linkages of inulin. Microbial production of inulinases, particularly from bacteria, is recommended due to their relatively rapid fermentation of substrates. *Bacillus* sp. is among the bacterial sources for inulinase. This study focused on the isolation, purification, and biochemical characterization of inulinase from *Bacillus* sp. produced through submerged fermentation of yacon. The crude inulinase was purified using ammonium sulfate precipitation, dialysis, and anion exchange chromatography on DEAE Sepharose FF achieving a 31.4-fold purification with a specific activity of 535.7 U/mg. The purified inulinase exhibited a K_m of 0.08 mM and a v_{max} of 255.9 µmoL/min, respectively, indicating a high affinity for its substrate. Characterization studies revealed an optimum pH of 5.0, with the enzyme retaining of 72-100% of its relative activity at the pH range of 3.5-6.0. The enzyme exhibited thermostability with 97% residual activity and 74% residual activity at 4 ºC and 37 ºC, respectively, at 4 days of incubation. The half-life of the enzyme at 50 ºC was determined to be 115 minutes. These findings revealed that purified inulinase could be used to produce fructose and potential fructooligosaccharides, with promising applications in the food industry.

Keywords: *Bacillus* sp.; enzyme purification; inulinase; submerged fermentation; yacon

Natural Products, Biological Chemistry and Chemical Biology (NB-P-006)

Development of new microwave method for cannabidiol (CBD) and Δ^9-tetrahydrocannabinol (THC) production

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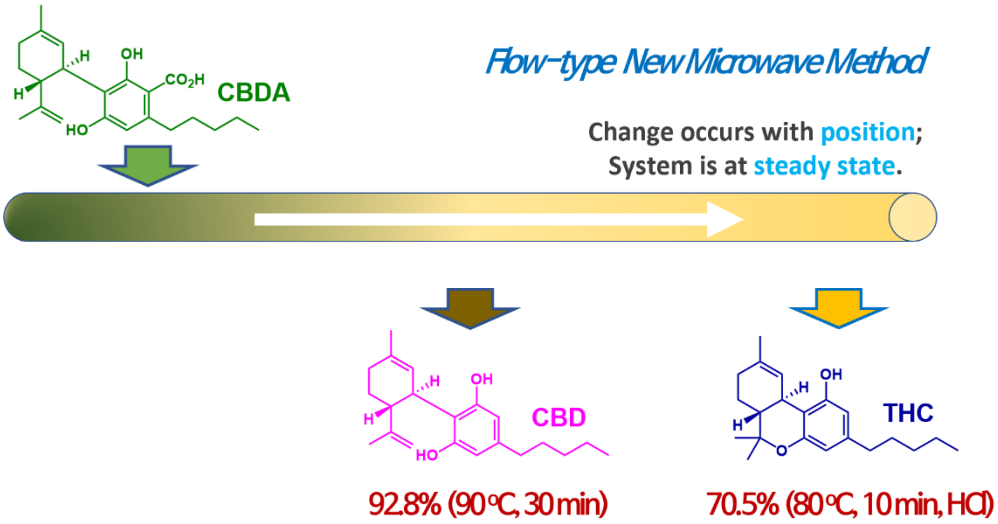
The global industrial hemp market is rapidly expanding, driven by the growing demand for cannabinoids such as CBD (cannabidiol) and Δ^9-THC (teterahydrocannabinol), highlighting the need for efficient production technologies. This study optimized CBD and Δ^9-THC production by combining dielectric heating-based microwave technology with a continuous process. For CBD production via CBDA decarboxylation in hemp extracts, the continuous process achieved a higher yield (92.8%) under milder conditions (90 °C for 30 min) compared to the batch process (90.3% at 120 °C for 30 min). Similarly, for Δ^9-THC production via CBD cyclization in hemp extracts, the continuous process yielded 70.5% under shorter reaction times (80°C for 10 min with HCl) compared to 62.1% in the batch process (80 °C for 20 min with *p*-toluenesulfonic acid). These results demonstrate that continuous microwave processing is an efficient and scalable technology for cannabinoid production, supporting the growth of the global industrial hemp market.

Keywords: industrial hemp; cannabinoids; cannabidiol; tetrahydrocannabinol; microwave



Natural Products, Biological Chemistry and Chemical Biology (NB-P-008)

Extraction of furfurals from coffee beans using deep eutectic solvents

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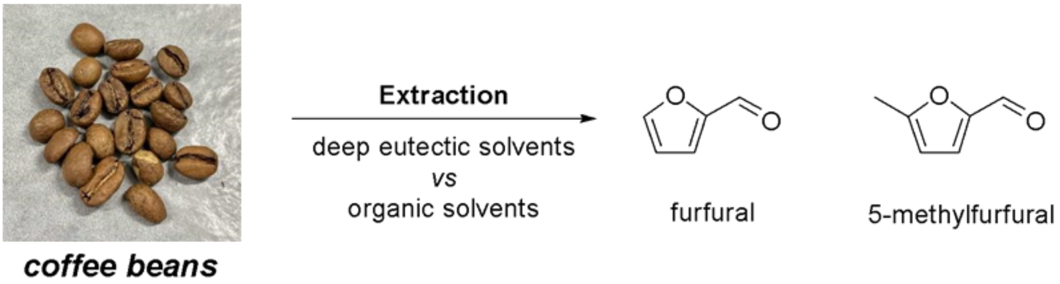
Furfural and 5-methylfurfural are volatile aromatic compounds abundantly found in coffee beans and have a sweet almond-like aroma. They are considered vital food constituents and are used in many products as fragrances in food, beverages, and cosmetics. The present study describes the use of low-toxicity solvents called deep eutectic solvents (DESs) for efficient extraction from coffee beans. Water and organic solvents, EtOH, 50% EtOH, acetone, and hexane, were used as control solvents to evaluate the extraction. Quantitative analysis was performed using gas chromatography-mass spectrometry (GC-MS) in selected ion monitoring mode. Scanning electron microscopy (SEM) for extracted samples was also conducted. The results demonstrated that extraction from coffee beans using arginine/L-lactic acid (molar ratio of 1:5) afforded the highest yield among DESs, at 0.014% and 0.0021% for furfural and 5-methylfurfural, respectively. The yield of furfural in water was 0.012%, and 5-methylfurfural in 50% EtOH was 0.0025%, which was almost the same as those of arginine/L-lactic acid. The results indicated that effective extraction from coffee beans under milder conditions than those needed for conventional methods. The use of less toxic and environmentally benign DESs for extraction would be applicable to the food and cosmetic industries.

Keywords: coffee; furfurals; extraction; deep eutectic solvents



Natural Products, Biological Chemistry and Chemical Biology (NB-P-009)

Correlation between LC-MS/MS and ELISA methods for quantitative analysis of desmosine-containing solutions

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Desmosine and isodesmosine are crosslinking amino acids found in extracellular matrix protein elastin, which imparts elasticity to tissues such as those of the lungs and arteries. These compounds are promising biomarkers for diseases involving elastin degradation, such as chronic obstructive pulmonary disease (COPD). This study examined the correlation between isotope-dilution LC-MS/MS and a newly established ELISA for *in vitro* diagnosis using a variety of samples. Results of LC-MS/MS and ELISA analyses exhibited a high correlation coefficient (0.9941). However, whereas the LC-MS/MS measurements deviated approximately 2-fold from theoretical values, the ELISA measurements ranged from 0.83 to 1.06 (average 0.94) times the theoretical values. Precise measurement of the absorbance of synthetic desmosine revealed a molar extinction coefficient of 2403, which differed markedly from the previously reported value of 4900 in 1963. Using this value to recalculate the amount of added desmosine, the LC-MS/MS measurements were 0.68 to 0.99 (average 0.87) times the theoretical values. Thus, the developed ELISA enables highly accurate determination of desmosine concentrations, comparable to LC-MS/MS, suggesting that ELISA is a potentially useful *in vitro* diagnostic tool.

Keywords: desmosine; LC-MS/MS; ELISA

Natural Products, Biological Chemistry and Chemical Biology (NB-P-015)

Biophysical studies of a serine protease domain in tissue plasminogen activator

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Ischemic stroke, which accounts for approximately 50% of cerebrovascular diseases, is caused by vascular blockage, while hemorrhagic stroke results from vessel rupture. Recombinant tissue plasminogen activator (r-tPA), the current standard thrombolytic agent, has a short half-life and requires high doses that increase bleeding risk. To overcome these limitations, we investigated the serine protease domain of tissue plasminogen activator (tPA-SPD) as a potential therapeutic candidate. tPA-SPD was isolated from an inclusion body, solubilized in a buffer, purified by His-tag affinity chromatography and dialyzed into PBS. The protein was then analyzed for enzymatic activity. The purified tPA-SPD showed stable solubility and retained serine protease activity, confirming its ability to interact with plasminogen. Enzymatic kinetics further demonstrated its significant proteolytic function, validating its structural integrity. These findings support the potential of tPA-SPD as a novel therapeutic agent for targeted plasminogen activation.

Keywords: human tissue-type plasminogen activator; plasminogen activator inhibitor; inclusion body; mild solubilization; specific enzyme activity

Natural Products, Biological Chemistry and Chemical Biology (NB-P-018)

Developing small molecules as α-L-iduronidase (IDUA) protein stabilizers toward mucopolysaccharidosis type I (MPS-I) disease

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Mucopolysaccharidosis type I (MPS-I) is a lysosomal storage disease caused by α-L-iduronidase (IDUA) deficiency, leading to the accumulation of glycosaminoglycans (GAGs). The recombinant human α-IDUA (rh-α-IDUA) protein drug via enzyme replacement therapy (ERT) helps reduce GAG accumulation but is costly and unstable. Co-administration of rh-α-IDUA with small molecular-based stabilizers, enables to enhance ERT effectiveness. Although our first-generation molecules can stabilize rh-α-IDUA, it doesn't work in the cell-based studying. The second-generation stabilizer, the *C*-glycosidic iduronic acid analogue ACK600, enables to stabilize rh-α-IDUA and reduce substrate accumulation in the cellular study. However, its potency remains to be improved through further structural modifications. In this work, we would like to develop the new synthetic routes to facilitate structure diversity, allowing to explore new stabilizers. Through our efforts to prepare the desired *C*-glycosidic iduronic acid-based scaffold, the key transformation, the C5-epimerization, has been systematically investigated. Fortunately, this step to solve the poor stereoselectivity observed in the flipping reaction has been overcome through the change of the C1-leaving group from the O-acetyl group to halogen such as bromide or fluoride. With this new synthetic route in hand, development of the third-generation of rh-α-IDUA stabilizers will be studied.

Keywords: mucopolysaccharidosis type I (MPS-I); lysosomal storage disease; α-L-iduronidase (IDUA); enzyme replacement therapy (ERT); protein stabilizers

Natural Products, Biological Chemistry and Chemical Biology (NB-P-019)

Harnessing bacterial peptidoglycan precursors to develop a label-free molecule target engagement strategy: A breakthrough of current limits to potentially explore new lipid II binders

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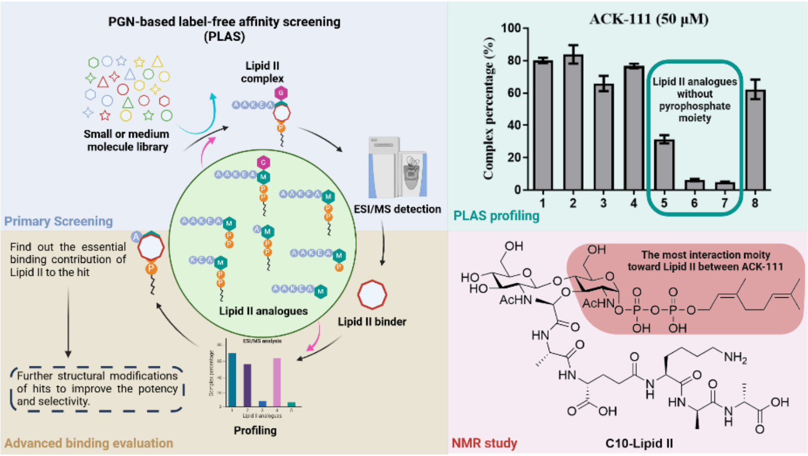
The rapid emergence of drug-resistant bacteria has become a serious threat. It is estimated that by 2050, more than ten million deaths per year could occur due to infections if urgent action is not taken. Peptidoglycan (PGN), a key component in bacterial survival, makes PGN biosynthesis an ideal target for developing antibiotics with fewer side effects. However, the enzymes involved in PGN biosynthesis exhibit a high mutation rate, impairing direct interactions between antibiotics and their targets. Therefore, increasing evidence suggests the need to shift focus toward targeting PGN-related biomolecules such as Lipid II. However, the development of inhibitors targeting Lipid II is challenging and time-consuming. Herein, we designed and synthesized Lipid II analogues as key chemical probes. Using these probes, we systematically optimized assay conditions to establish a rapid target engagement strategy called the PGN-based label-free affinity screening (PLAS) platform, which does not require tedious immobilization or labeling to measure binding affinity. PLAS enables efficient small-molecule screening to identify potent binders and further investigate the binding contributions of specific PGN moieties or fragments. The hit ACK-111 was identified from the pilot library screening, and its interactions with Lipid II via NMR studies showed the pyrophosphate of Lipid II plays an important role for interacting with ACK-111. More detailed information will be delivered in our poster.

Keywords: lipid II; peptidoglycan; antibiotic drug resistance; PGN-based label-free affinity screening; drug discovery



Dissecting the natural teixobactin to realize minimum structural requirements for binding bacterial Lipid II: Pilot studies of new antibiotics discovery

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Antibiotic-resistant pathogens are a growing global threat, making it crucial to find new strategies. Lipid II, a conserved precursor in peptidoglycan biosynthesis, is exposed on the bacterial outer membrane, making it a readily accessible antibiotic target. Natural antibiotics such as vancomycin, nisin, and teixobactin have been claimed as effective Lipid II binders, highlighting the therapeutic potential of this target. A previous study from our lab established the PGN-based label-free affinity screening (**PLAS**) platform, which enables the study of Lipid II interactions. In this work, 24 fragment-based analogues of teixobactin were designed and prepared. With these analogues in hand, we conducted binding studies using the **PLAS** assay to investigate their interactions with Lipid II. Among them, the tetracyclic peptide **CP-9** was identified as the minimal cyclic structure capable of strong binding, serving as a key component in targeting bacterial cell wall synthesis. Based on this minimal structure, we further explored modifications to enhance antimicrobial efficacy.

Keywords: antibiotic-resistant; peptidoglycan; lipid II; antibiotics; teixobactin

Development of a fluorescent polymyxin E-based probe to establish a fluorescence polarization (FP) platform for lipid A

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Due to the scarcity of novel antibiotics, polymyxin E has become a last-resort antibiotic for treating multidrug-resistant bacterial infections. Polymyxin E exerts its bactericidal effect by binding to the Lipid A component of lipopolysaccharides, thereby disrupting the bacterial membrane. However, the emergence of polymyxin E resistance and its nephrotoxicity highlight the urgent need to accelerate the discovery of new antibiotics. Unfortunately, convenient and effective platforms to facilitate this process are not currently available.

In this study, we isolated Lipid A and its resistance-modified variant [*Nat. Commun.* **2017**, *8*, 2054] from *Escherichia coli* and developed a novel fluorescence polarization (FP) platform [*Proc. Natl. Acad. Sci.* **2008**, *105*, 431–436]. Subsequently, Lipid A is conjugated to a fluorescent probe. Using the Cy5-labeled polymyxin E as a probe, we validated the platform by demonstrating its ability to detect competitive interactions between Lipid A-binding agents (such as polymyxins) and the probe for binding to Lipid A. We anticipate that this platform will contribute to the discovery of new antibiotics in the future.

Keywords: gram negative; fluorescence polarization

Pharmacokinetics and bioequivalence of ivermectin in dogs: A comparative study

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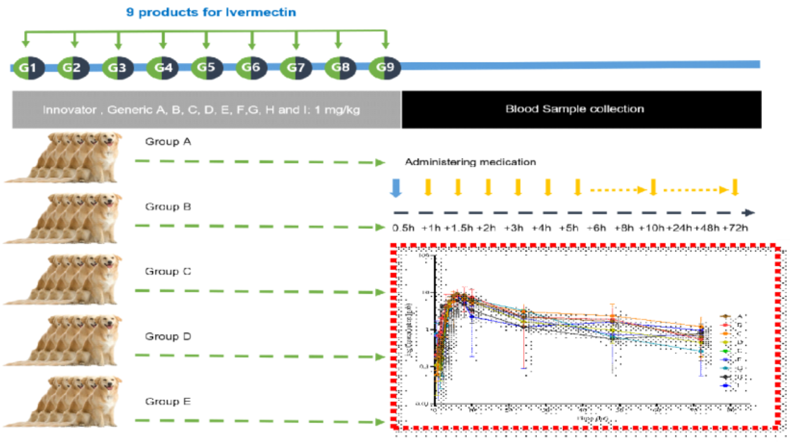
Ivermectin is a widely used, cost-effective antiparasitic drug for animals and humans, known for its efficacy and minimal side effects. This study aimed to evaluate the bioequivalence of nine commercially available ivermectin-containing topical formulations in dogs. Twenty-five clinically healthy Korean dogs (average weight: 14.3 kg) were divided into three groups: Control Innovator A and Test Generics B–I. Each formulation was topically administered at a dose of 6.0 µg/kg. Blood samples were collected at predetermined intervals and analyzed using liquid chromatography-tandem mass spectrometry (LC-MS/MS). Pharmacokinetic parameters, including time to maximum concentration (Tmax), maximum concentration (Cmax), and area under the curve over 24 hours (AUC24), were calculated for all formulations. The control product (Innovator A) showed a Tmax of 9.00 hours, a Cmax of 7.32 ng/mL, and an AUC24 of 260.74 hr*ng/mL. All generic formulations demonstrated pharmacokinetic values within the standard bioequivalence range of 80%–125% compared to the control product. These results confirm that all tested generic formulations are bioequivalent to the innovator product, ensuring comparable efficacy and safety profiles in clinical use. This study highlights the interchangeability of ivermectin generics and supports their continued use in veterinary medicine.

Keywords: ivermectin; bioequivalence; pharmacokinetics; Tmax; AUC values; korean dogs



Natural Products, Biological Chemistry and Chemical Biology (NB-P-025)

Establishing the cell-based metabolic assay platform to quantitatively measure heparan sulfate accumulation toward mucopolysaccharide storage disorders

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Heparan sulfate (HS) accumulation is an important pathogenic polysaccharide-typed biomarker for several mucopolysaccharides (MPSs). However, its varied polymeric lengths and sulfation patterns cause problems to easily and quantitatively measure the accumulated HS oligosaccharides. To the best of our knowledge, the MPS cell-based assay platform for small molecule library screening to easily readout the accumulation degree of HS oligosaccharides has not been extensively studied and established. In this study, the chemical digestion approach was applied through systematic analysis and the variant factors included different temperatures, solvents, and acids. Through our efforts, the trends and optimized conditions were sieved out. Meanwhile, the hydrolyzed fragments we discovered could not only serve as an analytic biomaker, but also guide us to design and prepare a surrogate. Indeed, our results showed that the qualified disaccharide-based surrogate, containing a glucosamine and uronic acid, can be added into analytic samples before acidic hydrolysis. Importantly, the coefficient of variance (CV) value could improve significantly form 15–43% to 7–14%. This cellular assay platform with a new developed surrogate is suitable to a pilot screening study of small molecule libraries in the future, which might accelerate the development of the substrate reduction therapy (SRT) toward MPS diseases.

Keywords: mucopolysaccharide storage disorders; heparan sulfate; diagnosis; screening

Natural Products, Biological Chemistry and Chemical Biology (NB-P-028)

The effect of prolidase expression in resistance of MCF7 breast cancer cells to chemotherapy

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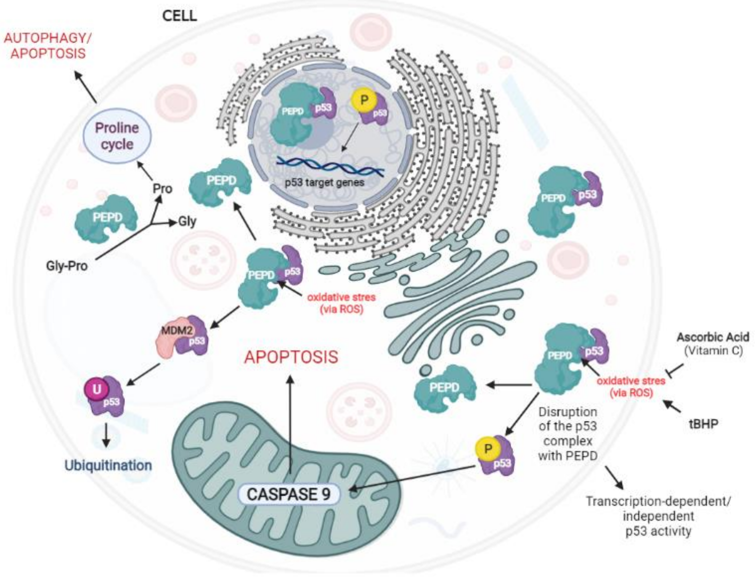
Tumor resistance to chemotherapy is a cause of treatment failure. One of the molecular reasons for this phenomenon may be the level of intracellular prolidase (PEPD). PEPD can bind and inhibit p53, blocking chemotherapy-induced apoptosis. The aim of this study was to investigate the activation of p53-dependent apoptosis activation in breast cancer cells with different PEPD levels: wild-type MCF7, PEPD-overexpressing MCF7 (MCF7^{PL}), and a zebrafish model. Doxorubicin (a direct activator of p53) induced apoptosis in the MCF7 cell and zebrafish xenografts dose-dependently, but less effectively in MCF7^{PL} cells, suggesting that PEPD overexpression prevents p53-dependent apoptosis. However, induction of oxidative stress (t-BHP) increased apoptosis, especially in MCF7^{PL}, an effect that was counteracted by Vitamin C. This suggests that a combination therapy involving a p53-dependent apoptosis inducer and an oxidative stress inducer may be a potential strategy for tumors with PEPD overexpression. The molecular mechanism of apoptosis induction under the conditions in tested models was associated with increased expression and translocation of p53 and increased expression of active forms of caspases 9 and 7. This was accompanied by decreased in DNA biosynthesis and mitochondrial potential, further supporting the role of oxidative stress in sensitizing PEPD-overexpressing cells to apoptosis.

Keywords: prolidase; chemotherapy resistance; cancer; p53



Natural Products, Biological Chemistry and Chemical Biology (NB-P-030)

Infusion of crushed Indonesia salam leaves (*Syzygium polyanthum*): Potential antihypercholesterol candidate_

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Cardiovascular disease is the leading cause of death globally, claiming about 17.9 million lives annually, which is 32% of all deaths. Statins can lower cholesterol but can cause liver damage and muscle pain. A study looked into natural alternatives using salam leaves. These leaves contain flavonoids, tannins, and saponins, which may lower cholesterol by stopping LDL oxidation, improving lipid metabolism, and reducing fat absorption. The research used 40 male Wistar rats on a high-fat diet for 14 days to increase cholesterol levels. The rats were then divided into five groups: one group received no treatment (negative control), one group received simvastatin (10 mg/kgBW) as a positive control, and three groups were given different doses of salam leaf decoction (0.52%, 0.72%, and 0.92%). Salam leaf decoction was administered for seven days through a tube, and cholesterol levels were measured using Point-of-Care Testing (POCT). The study revealed that the negative control group, which received no treatment, showed minimal effects. The positive control group treated with simvastatin (10 mg/kgBW) displayed positive results. Furthermore, three groups treated with salam leaf decoction at different doses (0.52%, 0.72%, 0.92%) showed significant effects, which increased with higher doses of salam leaf.

Keywords: Indonesia salam leaf; infusion of crushed leaf; antihypercholesterol; natural alternative therapies

Natural Products, Biological Chemistry and Chemical Biology (NB-P-031)

Biological evaluation of gallic acid–DMC hybrid derivatives against human lung cancer cell lines

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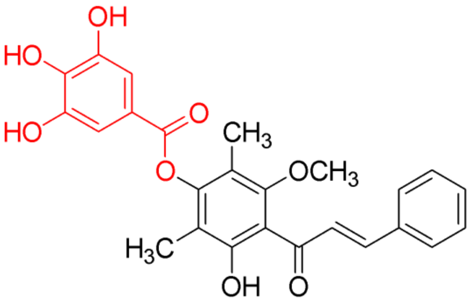
Lung cancer is the most prevalent malignancy and the leading cause of cancer-related deaths worldwide. Chalcones isolated from *Syzygium nervosum* A. have shown promising anticancer properties. The major compound 2′,4′-dihydroxy-6′-methoxy-3′,5′-dimethylchalcone (DMC or **1**) has shown cytotoxic activity against a variety of cancer cell lines. Structural modification of DMC by conjugating with gallic acid (**2**) may increase the anticancer effects. This project investigated the anti-lung cancer activity of the gallic acid–DMC hybrid derivative (**3**) as a potential anticancer agent. Compound **3** exhibited antiproliferative activity against NCI-H460 and A549 cells, with IC_{50} values of 3.93 ± 0.47 and 4.88 ± 1.42 µM, respectively. Notably, it displayed lower toxicity in MRC-5 normal cells, with an IC_{50} value of 10.48 ± 1.83 µM. Due to its higher potency in NCI-H460 cells, further analysis focused on apoptosis induction and mRNA expression. Treatment of NCI-H460 cells with compound **3** resulted in a three-fold increase in apoptotic cell death compared to control groups, as determined by the apoptosis assay. This compound showed anticancer activity by downregulating *AKT1*, *PDPK1*, *PTGER4*, and *PRKCA*, leading to PI3K/Akt pathway inhibition as confirmed by mRNA expression analysis. Our findings suggest that compound **3** is a promising candidate for anti-lung cancer drug development.

Keywords: lung cancer; gallic acid–DMC hybrid; antiproliferative activity; apoptosis; PI3K/Akt pathway



Compound **3**

Natural Products, Biological Chemistry and Chemical Biology (NB-P-032)

An efficient potential of amino acids conjugated with dimethylcardamonin–targeted inhibition of triple–negative breast cancer

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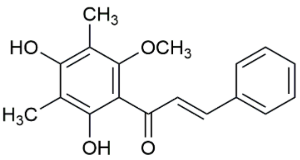
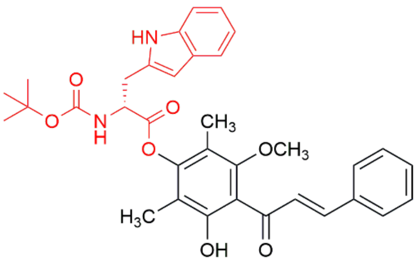
Triple-negative breast cancer (TNBC) represents an aggressive pathology of the breast cancer subtype. Chemotherapy is mainly conventional therapy for breast cancer; however, continuous use of chemotherapy treatment has frequently led to therapy resistance and recurrence in advanced-stage treatments. In this study, dimethylcardamonin (**1**) was isolated from seed of *Syzygium nervosum* A. Cunn. ex DC. To enhance anticancer activity of compound **1** on MDA-MB-231 triple-negative breast cancer cell line, it was structurally modified by conjugating with *N*-Boc-L-tyrosine to afford the novel 2′-hydroxy-4′-(*N*-Boc-L-tyrosinyloxy)-6′-methoxy-3′,5′-dimethylchalcone (**2**). Compounds **1** and **2** exhibited significant potential anti-proliferation with IC_{50} values of 14.54 ± 0.98 and 6.89 ± 0.85 μM, respectively, and showed low toxicity on Hs 578Bst normal cells. The most effective significant finding is that compound **2** revealed in terms of DNA damage on the MDA-MB-231 cell line, which was greater than compound **1** in a time-dependent manner. In addition, compound **2** can potentially increase sub-G0/G1 accumulation and arrests the G2/M phase of the cell cycle. Compound **2** induced apoptosis and cell death through the mitochondria-mediated intrinsic apoptotic pathway, as evidenced by a significantly decrease in mitochondrial membrane potential at the highest concentration. These results suggest that the novel compound **2** has potential as a promising anticancer candidate for the treatment of breast cancer.

Keywords: triple–negative breast cancer; anti-breast cancer; dimethylcardamonin; amino acids conjugated; chalcone derivatives



Dimethylcardamonin or DMC (**1**)



2′-hydroxy-4′-(*N*-Boc-L-tyrosinyloxy)-6′-methoxy-3′,5′-dimethylchalcone (**2**)

Natural Products, Biological Chemistry and Chemical Biology (NB-P-033)

Proteomic analysis reveals the intracellular mechanisms of human peripheral blood mononuclear cells-derived circulating proangiogenic cells differentiation after *ex vivo* treatment of iron-quercetin complex

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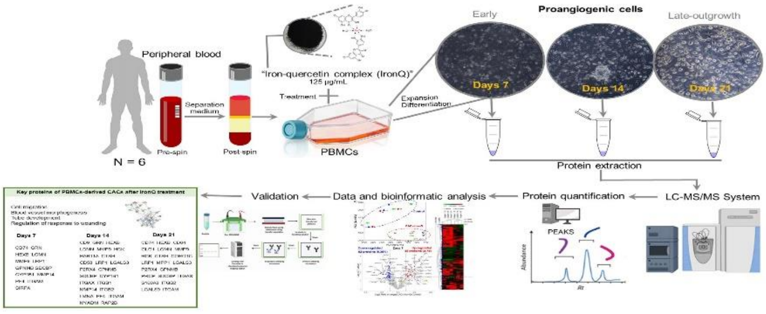
Cell-based therapies are a promising treatment for regenerative medicine using various classes of stem cells in revascularization. The role of peripheral blood mononuclear cells (PBMCs)-derived early endothelial progenitor cells (EPCs) is known as a circulating proangiogenic cell (CACs) in vascular repair of ischemic area. Our previous studies, iron(III)-quercetin complex referred to as IronQ, was synthesized with paramagnetic properties for MRI-based cell labelling and solubility. The major impact of IronQ (125 μg/mL) promoted human PBMCs differentiation into CACs with non-toxic and without adding specific growth factors of long cultivating time. To investigate differentiation changes, proteomics was applied to understand intracellular mechanisms from 7, 14 and 21 days using LC/MS-MS. The abundance of proteins associated with angiogenic effects was higher on day 7 and 14 compared to day 21. The pathway analysis of 8 up-regulated proteins were identified in vasculature development (GRN, LRP1, C3, GPNMB, CYP1B1, MMP14, PF4, ANPEP) in day 7 and 14 proteins (GRN, MYDGF, CTSH, LRP1, CHI3L1, GPNMB, CYP1B1, ITGAX, ITGB1, MMP14, ITGB2, PF4, ANPEP, HPSE) in day 14. These regulatory proteins played a vital role in angiogenic potential. This finding could be associated with understanding of several proteins of new insights in angiogenic properties after IronQ treatment.

Keywords: proteomics; molecular mechanisms; iron(III)-quercetin complex; circulating proangiogenic cells; peripheral blood mononuclear cells



Organic Synthesis and Medicinal Chemistry (OM-P-002)

Molecular basis of antitumor activity of novel platinum(II) bis(thiosemicarbazone) complex in breast cancer cells

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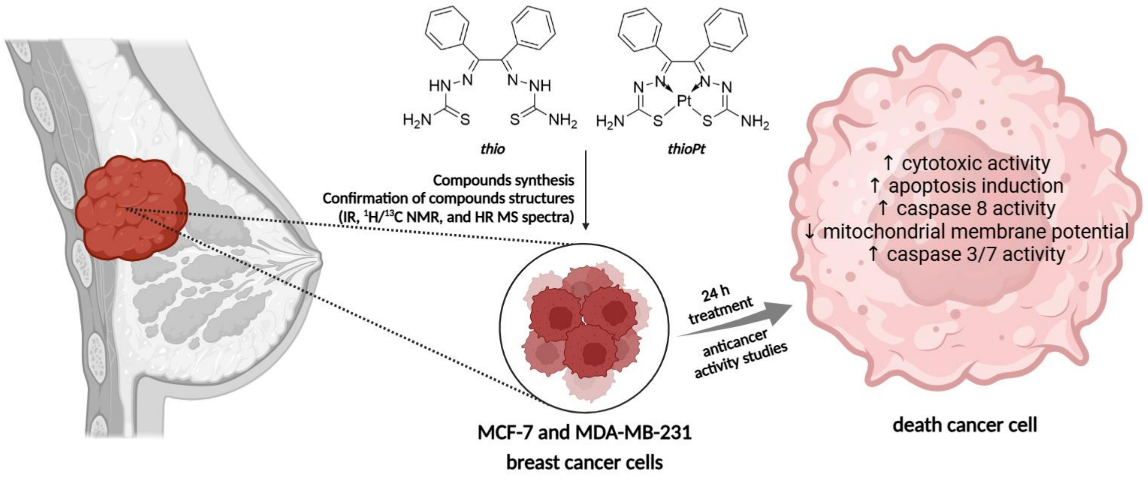
Disturbing cancer incidence rates, coupled with the resistance and toxicity of traditional anticancer drugs, hinder effective chemotherapy. Modern oncology seeks new, potent chemotherapeutics to address these challenges. Hydrazine derivatives, such as thiosemicarbazones, offer promise due to their nitrogen and sulfur atoms, which enable metal ions complexation and yield selective compounds with potent biological properties.

In the present study, a new platinum-based bis(thiosemicarbazone) derivative (thioPt) was synthesized and its anticancer properties against MCF-7 and MDA-MB-231 breast cancer cells were evaluated. The cytotoxic activity of the novel complex was examined using the MTT method of Carmichael [*Cancer Res.* **1987**, *47*, 936–942]. Cell viability studies showed that novel complex exhibited higher cytotoxic activity than cisplatin in MCF-7 and MDA-MB-231 and lower cytotoxicity in normal human breast epithelial cells (MCF-10A). Flow cytometry revealed that thioPt increased apoptotic cell counts and selectively accumulated in tumor mitochondria, enhancing its proapoptotic effects. Further analysis showed that thioPt induced apoptosis via both extrinsic and intrinsic pathways, activating caspase 8, reducing mitochondrial membrane potential, and increasing caspase 3/7 activity. These results indicate that novel platinum(II) bis(thiosemicarbazone) complex may be a suitable structure for the development of a new drug for breast cancer therapy and constitute a novel class of compounds with potential anticancer activity.

Keywords: thiosemicarbazones; platinum(II); breast cancer; anticancer drugs; apoptosis



Organic Synthesis and Medicinal Chemistry (OM-P-006)

Senotherapeutic effect of novel 1,2,4-triazine derivative in human colon cancer

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Cellular senescence plays a crucial role in tumorigenesis and is recognized as a hallmark of colorectal cancer. Emerging evidence suggests that 5-fluorouracil (5-FU)-induced senescence may contribute to chemoresistance and tumor recurrence. In this study, we examined the effects of 5-FU on colon cancer cell senescence and investigated whether novel 1,2,4-triazine derivative methyl 4-hydroxy-1-[4-(7-methyl-5*H*-pyrazolo[4,3-e]tetrazolo[4,5-b][1,2,4]-triazin-5-yl)phenylsulfonyl]-pyrrolidine-2-carboxylate (MM-129) could counteract its activity. Senescence was identified through the expression of senescence-associated β-galactosidase (SA-β-gal) using microscopy-based techniques, flow cytometry analysis, and immunohistochemistry staining. Additionally, we assessed the levels of interleukin-6 a key marker of the senescence-associated secretory phenotype (SASP).

To further elucidate MM-129's mechanism of action, we evaluated the SIRT1/STAT3 signaling pathway. Our findings demonstrated that MM-129 effectively counteracted 5-FU-induced senescence in colon cancer cells and dramatically decreased the proportion of senescent cells in DLD-1 and HT-29 from 69% to 29% ($^{\wedge\wedge\wedge}p<0.001$ vs 5-FU) and from 55% to 17% ($^{\wedge\wedge\wedge}p<0.001$) respectively. Moreover, MM-129 inhibited senescence by reducing SASP factor (IL-6). Through modulation of the SIRT1/STAT3 pathway, MM-129 induced the selective elimination of senescent cells.

Our study suggests that MM-129 acts as a novel senolytic agent and that targeting STAT3 could be a potential strategy for selectively eliminating senescent cells. Combining cancer therapies with senolytics may enhance therapeutic outcomes and open new avenues for cancer treatment.

Keywords: 1,2,4- triazine derivative; cellular senescence, senescence-associated secretory phenotype; xenograft; colon cancer

Organic Synthesis and Medicinal Chemistry (OM-P-007)

Ag-gC_3N_4 as heterogeneous photocatalysts for copper-free azide-alkyne cycloaddition reactions

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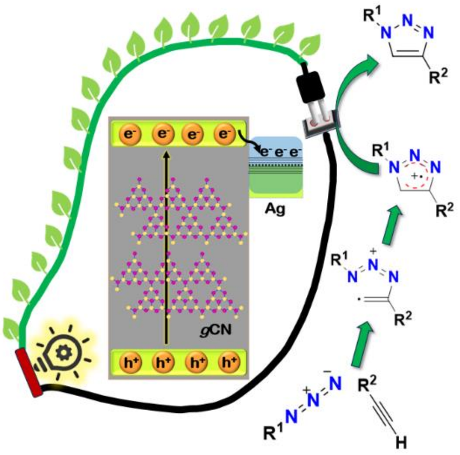
A novel and sustainable photocatalytic system for copper-free azide-alkyne cycloaddition (AAC) reactions have been demonstrated, affording 1,4-disubstituted 1,2,3-triazoles at room temperature. Unlike traditional approaches, which often rely on copper catalysts and face issues such as unwanted by-products and metal contamination, this method employs a novel visible-light-active heterogenous photocatalyst comprised of nanostructured Ag and graphitic carbon nitride (*g*CN). It exhibits improved visible-light absorption properties due to a reduced band gap facilitated by the introduction of Ag nanoparticles. It was synthesized by immobilizing silver nanoparticles onto *g*CN, enabling highly efficient and 100% regioselective production of 1,4-disubstituted 1,2,3-triazoles at room temperature. The catalyst operates via a single-electron transfer (SET) mechanism, distinct from traditional metal acetylide coordination pathways, highlighting the crucial role of light in achieving excellent results. This was experimentally confirmed through quenching experiments using various radical scavengers. Sustainability assessments validated the greenness of our catalytic route, revealing a 100% atom economy, low environmental factor (E-factor), a high eco-scale score and high reaction mass efficiency (RME). The catalyst demonstrated excellent reusability, maintaining consistent yield over at least five cycles. This innovative approach represents a significant advancement in green chemistry, offering a sustainable, versatile, and efficient alternative for a broad range of substrates in AAC reactions, having advantages over most of the recently reported protocols involving state-of-the-art copper-free heterogeneous photocatalysts.

Keywords: photocatalyst, azide-alkyne cycloaddition, visible light, copper-free, graphitic carbon nitride.



Organic Synthesis and Medicinal Chemistry (OM-P-008)

In-silico study of dibenzylidine-cyclohexanone curcumin analogs as potential Inhibitors of *Mycobacterium tuberculosis* protein PASTA kinase PkB (PknB)

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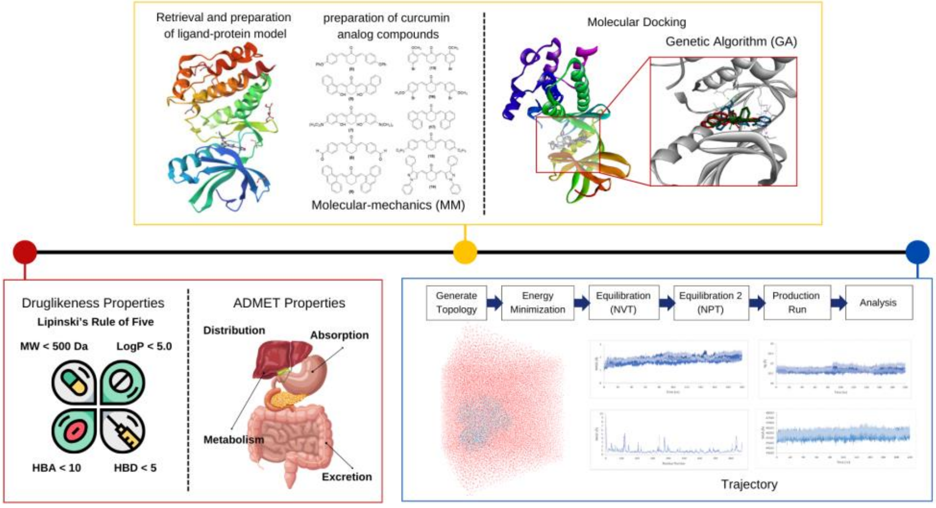
Mycobacterium tuberculosis (M. tb) PASTA kinase PkB (PknB) is a transmembrane protein, crucial for cell survival. It has a role in metabolism, cell division, and cell wall synthesis, making it a potential drug target for tuberculosis. This study aims to predict the antituberculosis potential of dibenzylidine-cyclohexanone curcumin analog compounds as inhibitors of PknB of M. tb. This study used ten curcumin analog compounds and the crystal structure of M. tuberculosis PASTA kinase PknB (PBD ID: 5U94). Druglikeness and ADMET evaluations were conducted using the pkCSM and ProTox II software. The molecular docking (MD) and Molecular dynamics simulations (MDS) were performed using Autodock 4.2 and Gromacs 2023. Virtual screening showed curcumin analogs are still within the ranges for each parameter, reasonably safe, and non-toxic. The MD results revealed that compounds A119, A109, and A106 are the top three with the lowest binding energy (–11.38; –10.79; and –10.23 kcal/mol, respectively) than curcumin and mitoxantrone as one of the anti-mycobacterial agent (–9.06 and –9.62 kcal/mol). The MDS showed flexibility, deformability, and stability of well-docked complexes with RMSD, RMSF, Rg, SASA, Hbond, and MM-PBSA. In conclusion, this study revealed a novel antiTB substance that inhibits the Protein PASTA PKnB.

Keywords: curcumin analogs; molecular docking; protein PknB; *in-silico*; antituberculosis



Organic Synthesis and Medicinal Chemistry (OM-P-012)

Oxidation reactions in water using copper catalysts covalently tethered on a thermo-responsive polymer

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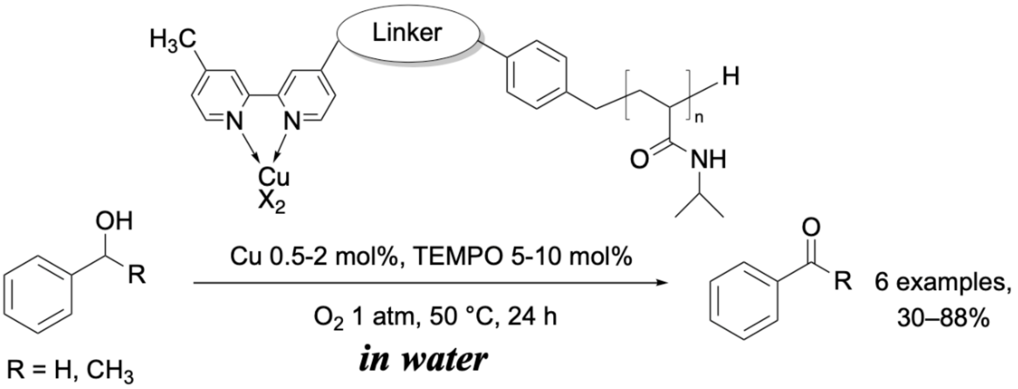
Water is an attractive reaction solvent with low environmental impact because of its low toxicity and abundance. Considering the shift to environmentally benign processes in the future, it is of significance to study catalytic reactions in water. We have been studying application of thermo-responsive polymer for organic synthesis in water. In particular, poly(*N*-isopropylacrylamide) (PNIPAAm), which has lower critical solution temperature (LCST) at 32 °C, is attractive material because it provides hydrophobic circumstance in water at higher temperature, while it dissolves in water at room temperature. We envisioned that PNIPAAm might allow more effective organic reactions in water and/or efficient extraction of the product.

In this study, we report copper catalysts tethered on a thermo-responsive polymer which are useful for oxidation reactions in water. Bipyridyl moiety was covalently tethered on a reversible addition-fragmentation chain transfer (RAFT) agent by copper-catalyzed cycloaddition. *N*-Isopropylacrylamide was polymerized using this RAFT to afford a polymer in which the bipyridyl ligand is covalently immobilized at the terminus of each polymer chain. Copper complex was prepared using the polymer and copper-catalyzed oxidation reaction of 1-phenylethanol was performed in water. Extraction with ethyl acetate from the reaction mixture afforded acetophenone in 30-88% yield. The product yields depended on catalyst and TEMPO loading.

Keywords: copper; catalyst; reaction in water; thermo-responsive polymer; poly(*N*-isopropylacrylamide)



Organic Synthesis and Medicinal Chemistry (OM-P-014)

Carboxylate-directed palladium-catalyzed regioselective Mizoroki−Heck alkenylation of γ,δ-unsaturated carboxylic acids

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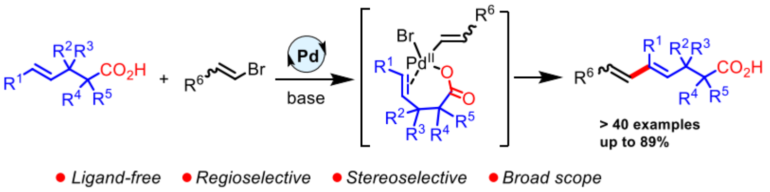
This study reports a novel and efficient approach to the carboxylate-directed palladium-catalyzed Mizoroki-Heck alkenylation of γ,δ-unsaturated carboxylic acids with alkenyl bromides, highlighting its potential in organic synthesis. The incorporation of a carboxylate group proves to be an excellent strategy for facilitating chelation to the palladium center, thereby promoting regioselectivity and control over the reaction pathway. This method enables the distal alkenylation of electronically unbiased internal alkenes, leading to the formation of conjugated 1,3-dienes with remarkable high stereoselectivity. Notably, the synthetic utility of these conjugated 1,3-diene products is extensive; they can be further transformed through a variety of chemical reactions, including reduction to yield 1,3-dienyl alcohols, epoxidation to form epoxides, methylation to introduce methylester groups, amidation to create amides, and cycloaddition to generate complex cyclic structures. Overall, this work not only advances the field of carboxylate-directed Mizoroki-Heck reactions but also opens new avenues for the utilization of versatile conjugated diene systems in innovative synthetic applications [*Adv. Synth. Catal.* **2023**, *365*, 699–703].

Keywords: carboxylate-directed; palladium-catalyzed; Mizoroki-Heck; alkenylation; conjugated 1,3-dienes



Organic Synthesis and Medicinal Chemistry (OM-P-015)

Synthesis of 2-aroylchromones catalyzed by *N*-heterocyclic carbenes

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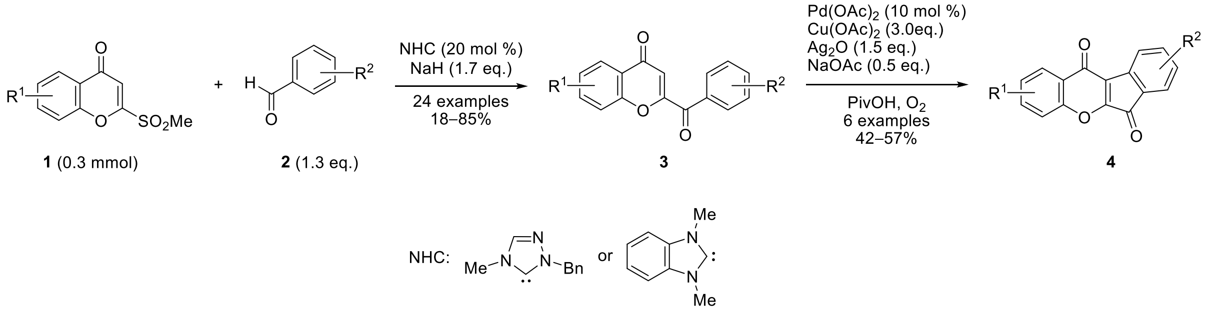
For their bioactivities and versatility, 2-aroylchromones are attractive motifs in synthetic organic chemistry. Nonetheless, there has been no reported method for the direct introduction of various aroyl groups at position 2 of chromones. Thus, we investigated the aroylation of 2-(methylsulfonyl)chromones catalyzed by *N*-heterocyclic carbenes (NHCs), where the sulfonyl group was used as a leaving group and aromatic aldehydes as aroyl group sources.

The reaction of quinolone **1a** (R^1 = H) with benzaldehyde **2a** (R^2 = H) in the presence of NaH using azolium salts as NHC precursors successfully afforded aroyl chromone **3a** ($R^1 = R^2$ = H). The reaction proceeded most efficiently when triazolium salts were used in acetonitrile. Aromatic aldehydes with either electron-donating or electron-withdrawing groups and heteroaromatic aldehydes were tolerated in the reaction, affording the corresponding **3**. The use of the aza-substrate, 1-methyl-2-quinolone, was also examined.
As a synthetic application, compounds **3** were used in the synthesis of anticancer compound wrightiadione **4a** ($R^1 = R^2$ = H) and analogues of it. The resulting products **4** demonstrate the synthetic utility and importance of the 2-aroylchromones **3**.

Keywords: chromone; *N*-heterocyclic carbene; organocatalysis; aroylation; wrightiadione



Organic Synthesis and Medicinal Chemistry (OM-P-016)

Iridium-catalyzed C–H borylation; diverse selectivity depending on ligand structure

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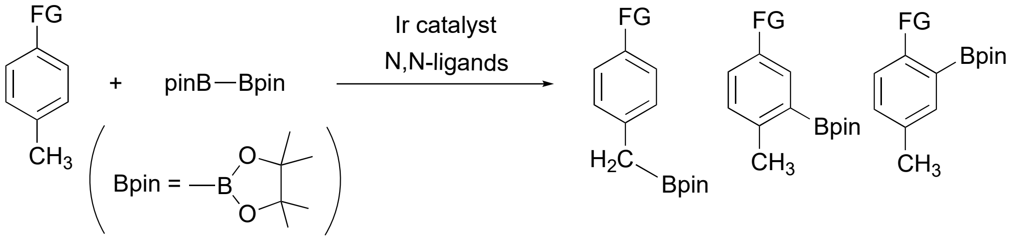
Transition metal-catalyzed functionalization by activation of C-H bonds have attracted much attention from the viewpoint of atom economy. Since the first report of borylation reactions with iridium complexes by Ishiyama, Miyaura and Hartwig [*J. Am. Chem. Soc.* **2002**, *124*, 390–391], much effort has been focused on the development of regioselective borylation. In particular, there have not been many reports on selective borylation of sp^3 carbon at the benzyl position, and issues remain, such as the use of excessive substrates. In this study, borylation reactions were investigated for aromatic compounds with methyl groups using various N,N-bidentate ligands other than the bipyridyl skeleton. We employed various toluene derivatives with a functional group at *p*-position. When those have an electron-withdrawing group was used, borylated products were obtained in good yields, whereas those with an electron-donating groups resulted in poor yields. Interestingly, reactions using pyridyltriazole ligands predominantly afforded benzyl-borylated products. On the other hand, pyridyloxazole ligands selectively provided ortho-borylated products.

Keywords: C-H activation; borylation; iridium catalyst; *N*,*N*-ligand



Organic Synthesis and Medicinal Chemistry (OM-P-018)

Iridium-catalyzed decarbonylative annulation of benzoic pivalic anhydrides with alkynes

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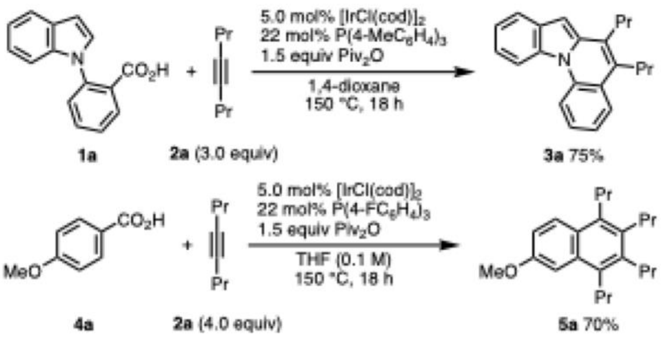
The synthesis of polycyclic aromatic compounds is a critical area of research due to their diverse applications as key intermediates in organic semiconductors and luminescent materials. Among the various synthetic strategies, transition-metal-catalyzed benzannulation stands out as one of the most straightforward 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 $P(4\text{-}MeC_6H_4)_3$ (22 mol%), the desired annulation product, indolo[1,2-*a*]quinoline (**3a**), was obtained in a 75% isolated yield. Similarly, the reaction of 4-methoxybenzoic acid (**4a**) with **2a** and pivalic anhydride under analogous conditions afforded 6-methoxy-1,2,3,4-tetrapropylnaphthalene (**5a**) in a 70% isolated yield.

Keywords: iridium; annulation; aromatic compounds; anhydrides; decarbonylation



Organic Synthesis and Medicinal Chemistry (OM-P-022)

IsoChichibabin/Chichibabin pyridinium syntheses of desmosine/isodesmosine-$^{13}C_3$,$^{15}N_1$

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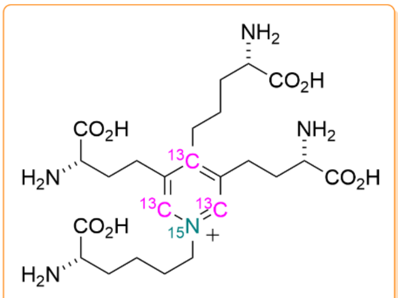
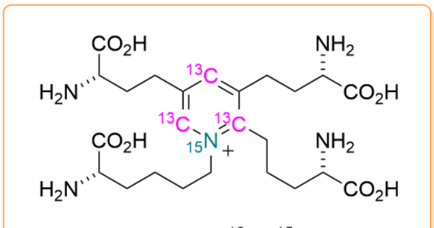
Pyridinium amino acids desmosine and isodesmosine are crosslinking amino acids of elastin that contributes to elasticity of ligaments, skin, etc. They are expected to be biomarkers for diseases associated with elastin degradation. In this study, syntheses of internal standards desmosine-$^{13}C_3$,$^{15}N_1$ (**1**) and isodesmosine-$^{13}C_3$,$^{15}N_1$ (**2**) for quantitative LC-MS/MS analysis of desmosine and isodesmosine were targeted.

Starting from commercially available protected glutamic acid, the corresponding side chain aldehyde was synthesized in 6 steps. ^{13}C atom was then introduced by Wittig reaction followed by hydroboration-oxidation reaction and IBX oxidation, and protected allysine was synthesized. The bromo compound was synthesized in 5 steps from another protected glutamic acid. ^{15}N was introduced by the S_N2 reaction using $KC^{15}N$, and the protected lysine was synthesized by subsequent hydrogenation under high pressure. Lastly, Chichibabin pyridinium synthesis or isoChichibabin pyridinium synthesis was performed to form pyridinium and all protecting groups were removed to complete the syntheses of the target compounds. These compounds will be used for quantitive LC-MS/MS analysis of desmosines in bovine samples, such as oni-suji a kind of tendon, as internal standards.

Keywords: desmosine; isodemosine; elastin; LC-MS/MS; organic synthesis


desmosine-$^{13}C_3$,$^{15}N_1$ (**1**)


isodesmosine-$^{13}C_3$,$^{15}N_1$ (**2**)

Organic Synthesis and Medicinal Chemistry (OM-P-023)

Preparation of desmosine-carrier protein conjugated antigen aiming at antibody production

Mika Ryu, Mayu Kodaka, Reiko Yokoo, Toyonobu Usuki*
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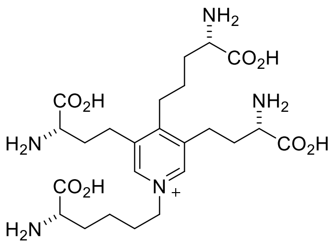
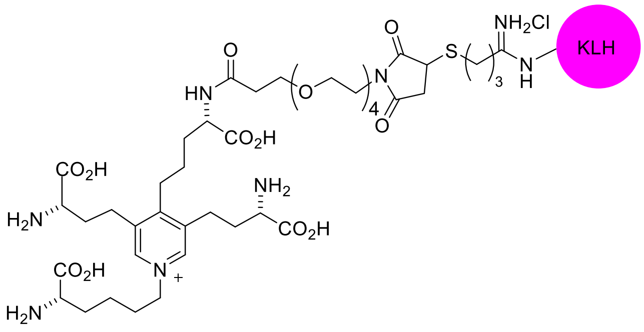
Desmosine is a major crosslinking amino acid of the elastic fiber elastin. Our laboratory has succeeded in first total synthesis of desmosine. Recently, quantitative analysis of desmosine in biological samples is desired to monitor diseases related to elastin degradation. ELISA, a method to detect the presence of antigens in samples, can be useful to detect desmosine. For the preparation of ELISA, we need desmosine-protein complex antigen since desmosine itself has no immunogenicity. In this study, we report the preparation of desmosine-protein complex antigen in which the carrier protein is bound to desmosine.Our established synthetic method for desmosine has been used for the synthesis of target compounds. Synthesis of trisubstituted pyridine was conducted by Sonogashira and Negishi cross-coupling reactions. Target compounds were synthesized via hydrogenation, intramolecular condensation, *N*-alkylation and Michael addition with thiolated KLH (Keyhole Limpet Hemocyanin). KLH was selected as the carrier protein because anti-desmosine antibodies were not produced when BSA (Bovine Serum Albumin) was used as the carrier protein.

Keywords: desmosine; ELISA; antigen; carrier-porotein; cross-coupling reaction



desmosine



KLH-conjugated desmosine (1)

Organic Synthesis and Medicinal Chemistry (OM-P-025)

Total synthesis of collagen immature crosslinker lysinonorleucine

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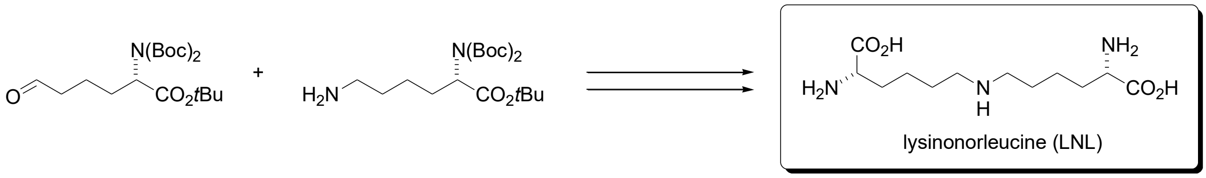
Collagen is a fibrous extracellular matrix protein and plays an essential role in skin elasticity, joint flexibility, and bone strength. It has a triple helix structure of three polypeptides and forms stable collagen fibers by covalent bonds. In collagen crosslinkers, dehydrolysinonorleucine (deH-LNL) is an immature crosslinker and considered to be a precursor of mature crosslinkers. Although immature crosslinkers exist in the whole body, a precise method of quantitative analysis has not been established yet. In this study, we achieved total synthesis of lysinonorleucine (LNL) by coupling between protected allysine aldehyde and protected lysine from commercially available protected glutamic acids. Further synthetic study including a labeled compound will be presented.

Keywords: collagen; crosslinker amino acids; lysinonorleucine



Organic Synthesis and Medicinal Chemistry (OM-P-026)

Synthesis of β-O-4 model compound labelled ^{13}C isotope of lignin

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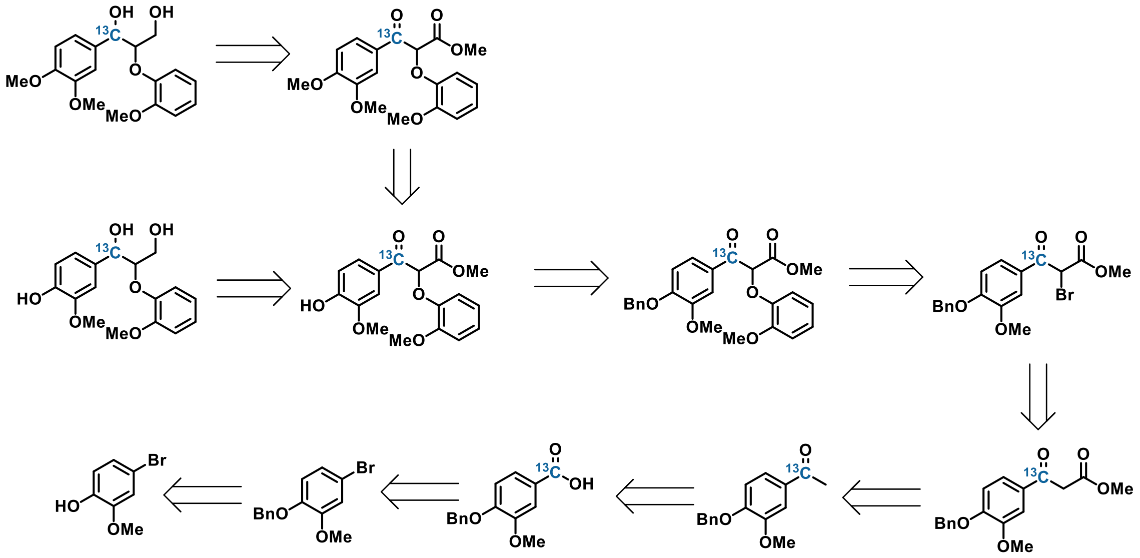
Lignin is a heterogeneous aromatic polymer, known for its complexity and amorphous structure. The reaction mechanism for lignin depolymerization remains poorly understood. Mechanistic study is currently challenging due to characterization of lignin. However, the β-O-4 linkage is the most prevalent, accounting for 45-75% of the total linkages in native lignin [*Renew. Sustain. Energy Rev*. **2019**, *107*, 232–249]. This research has developed the synthetic internal and terminal β-O-4 model compound including isotopically labelled variants to investigate key intermediates in lignin polymerization for mechanistic studies, leading to the reactivity of various linkages and development of methods to valorize biomass into value-added products.

Keywords: lignin; β-O-4 linkage; aromatic polymer; lignin polymerization



Organic Synthesis and Medicinal Chemistry (OM-P-028)

Design, synthesis, and evaluation of brominated biscoumarins as potent α-glucosidase inhibitors

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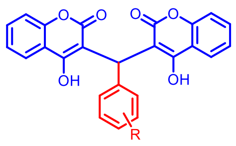
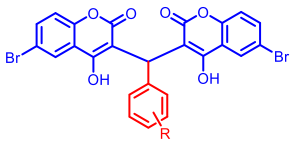
Diabetes is one of the most rapidly increasing diseases globally and is expected to affect 693 million adults by 2045. α-Glucosidase (AG) inhibitors such as acarbose, miglitol and voglibose are oral anti-diabetic drugs currently used to treat type 2 diabetes. However, the use of these drugs may increase the risk of hepatotoxicity and cause flatulence or diarrhea. Therefore, this study aims to synthesize potent compounds with high efficacy while minimizing side effects for diabetes treatment. Seventeen biscoumarin derivatives (**1–17**), including eight new compounds, were synthesized, and their AG inhibitory potentials were evaluated against AG from *Saccharomyces cerevisiae* E.C 3.2.1.20. The synthesized biscoumarins exhibited excellent inhibitory activity against AG (IC_{50} values ranging from 0.07 to 30.77 µM) compared to acarbose (IC_{50} = 93.63 µM). The results showed that brominated biscoumarin derivatives at C-6 and C-6' on the two coumarin rings (compounds **6**, **8–10**) demonstrated better inhibitory activity than their corresponding biscoumarin analogues derived from 4-hydroxycoumarin. In addition, brominated biscoumarin-1,2,3-triazole **17** was identified as the most potent inhibitor. The kinetic study of **17** revealed its competitive inhibitory nature toward AG (K_i = 1.13 µM). These findings suggest that biscoumarins containing bromine substituents on the 4-hydroxycoumarin ring and biscoumarin-1,2,3-triazoles could be promising candidates for further studies as anti-diabetic drug candidates.

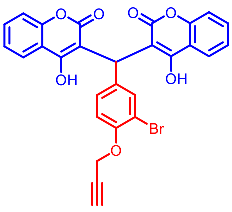
Keywords: biscoumarins; triazole; alpha-glucosidase; diabetes



1, R = H
2, R = 4-C_4H_9
3, R = 4-OCH_3
4, R = 3-OCH_3-4-OH
5, R = 4-NO_2



6, R = H
7, R = 4-C_4H_9
8, R = 4-OCH_3
9, R = 3-OCH_3-4-OH
10, R = 4-NO_2



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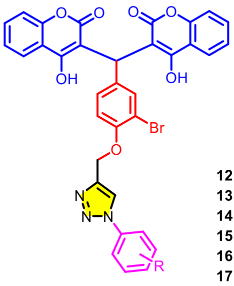

12, R = H;
13, R = 4-Br;
14, R = 2,4-diCl;
15, R = 3-OH;
16, R = 4-COOH;
17, R = 4-$CONH_2$

12-17

Organic Synthesis and Medicinal Chemistry (OM-P-029)

Direct Minisci-type C–H acylation of β-carbolines

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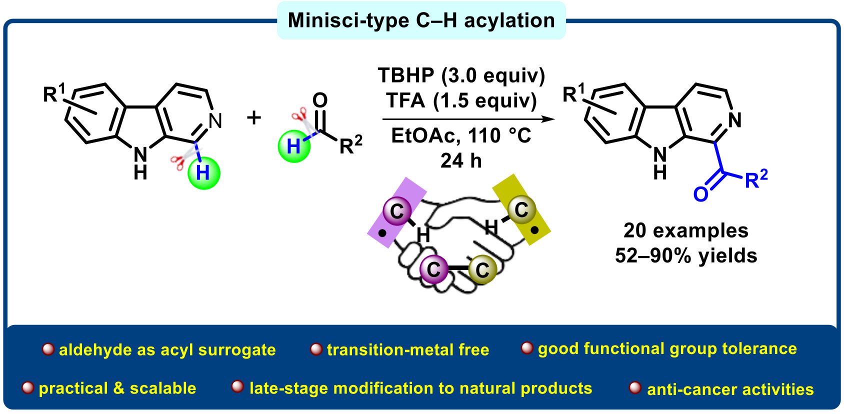
The direct C–H functionalization of β-carbolines via a Minisci-type radical process has received comparatively less attention than other electron-deficient *N*-heteroarenes such as pyridines, quinolines, isoquinolines, and pyrimidines. This is primarily due to the electron-deficient nature of the β-carboline core, compounded by potential electronic interference from the lone pair on the indole nitrogen. Additionally, the challenge for the synthesis of acylated β-carbolines persists due to inherent selectivity issues associated with existing synthetic procedures, leading to low yields of the desired products. To address these limitations, we developed a Minisci-type acylation of β-carbolines based on oxidative cross-dehydrogenative coupling (CDC) reaction with aldehydes. This metal-free C–H functionalization protocol is characterized by its simplicity, scalability, and applicability to late-stage functionalization, offering a valuable tool for the synthesis of biologically relevant β-carbolines, including natural product derivatives. Most impressively, *in vitro* anticancer screening against HepG2 liver cancer cells identified one compound with potent cytotoxicity, with activity competitive with that of clinical anticancer agent doxorubicin.

Keywords: β-carbolines; Minisci reaction; acylation; C–H functionalization; anticancer



Synthesis and antimicrobial activities of heterocyclic-chalcone analogs

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Arief Kusuma Wardani,[5] Erna Prawita Setyowati[6]
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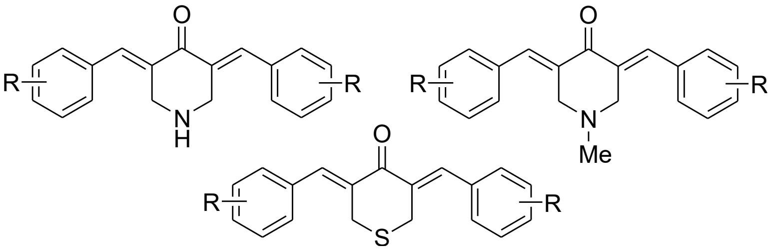
This study aimed to synthesise new heterocyclic-chalcone analogs and to test their activity as antimicrobial agents in Gram-positive, Gram-negative bacteria, and fungi. The heterocyclic-chalcone analogs in this research have a structure like chalcone with hetero-cyclicketone. These compounds are synthesised by using the Claisen-Schmidt condensation reaction, between aromatic aldehydes and tetrahydro-thiopyran-4-one, piperidin-4-one or 1-methylpiperidin-4-one. The reactions were conducted in acid or basic conditions, using HCl or NaOH as the catalyst. All compounds were then characterized using spectroscopic methods (IR, ^{1}H NMR, ^{13}C NMR) and MS. The compounds that were identified were tested for antimicrobial activity against *Staphylococcus aureus* (ATCC 25923), *Escherichia coli* (ATCC 25922), *Bacillus subtilis* (ATCC 6633), *Enterococcus faecalis* (ATCC 29212), *Klabsiella pneumoniae* (ATCC 13883), *Streptococcus mutans* (ATCC 25175), *Pseudomonas aeruginosa* (ATCC 27853) *and Candida albicans* (ATCC 10231) fungi using agar diffusion method indicated by the inhibition diameter of each compound. The results showed that moderate to high yields were obtained from the synthesis. Analog curcumin compounds showed antibacterial activity at concentration 62.5 µg/mL on Gram-positive bacteria and 125 µg/mL on Gram-negative bacteria. The compound containing two chlorine substituents on the benzene ring has better activity as an antimicrobial than other tested compounds.

Keywords: antibacterial; antimicrobial; antifungi; heterocyclic-chalcone analogs; synthesis



Organic Synthesis and Medicinal Chemistry (OM-P-032)

Structure modifications of macluraxanthone derivatives and their antioxidant and brine shrimp lethality activities

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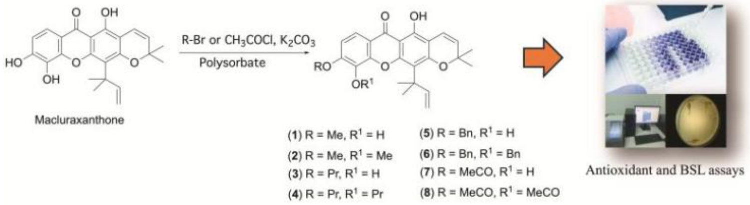
Macluraxanthone, a xanthone derivative, has been isolated from various plant sources, including *Garcinia schomburgkiana*. This compound exhibits a range of biological activities, such as antioxidant, anticancer, and antimicrobial properties. To explore its potential, a series of *O*-substituted macluraxanthone derivatives were synthesized via phase-transfer catalyzed alkylation using alkyl halides. The structures of these derivatives were characterized by spectroscopic techniques. All synthesized derivatives were evaluated for their antioxidant activity using DPPH (2,2-diphenyl-1-picrylhydrazyl) and ABTS (2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) assays, as well as their toxicity using the brine shrimp lethality assay (BSLA). The results demonstrated that macluraxanthone derivatives **2** and **5** exhibited significant antioxidant activity in both DPPH and ABTS assays. Furthermore, BSLA data indicated that all synthetic derivatives were non-toxic to *Artemia salina* larvae, with LC_{50} >1000 μM. These findings highlight the potential of macluraxanthone derivatives for further synthetic modification, biological evaluation, and structure-activity relationship (SAR) studies to optimize their pharmacological properties.

Keywords: Macluraxanthone; synthetic derivatization; antioxidant; toxicity



Organic Synthesis and Medicinal Chemistry (OM-P-035)

Efforts towards the synthesis of picrotoxane family

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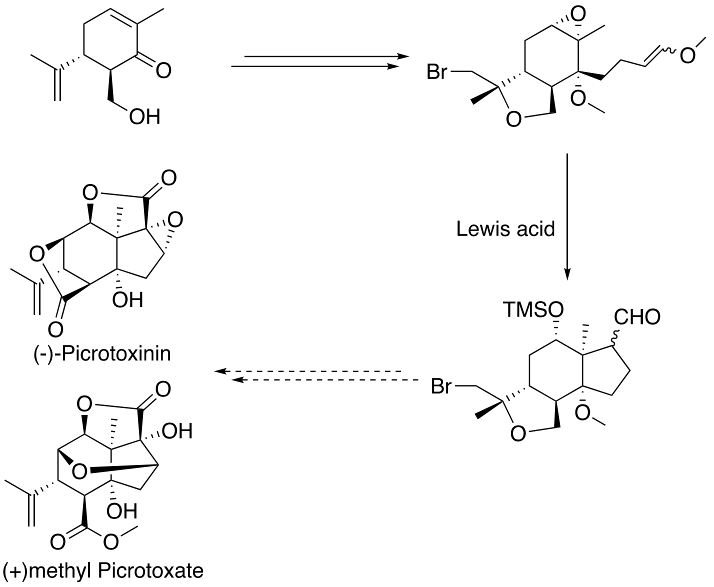
Picrotoxinin was isolated from the poisonous plant *Anamirta cocculus* in 1812. It has been identified as an inhibit of the chloride channel GABA$_A$ receptor as a non-competitive antagonist [*Chem. Rev.* **1967**, *67*, 441–464]. (–)-Picrotoxinin contains cis-fused hydrindane core with 8 continuous chiral centers also with 2 γ-lactone ring and an epoxide. To date, six group have published the total synthesis of (–)-picrotoxinin. A Lewis acid catalyzed cyclization had been well-developed [*Org. Lett.* **2015**, *17*, 3398–3401] and we adopted as a key ring formation process for the *cis*-fused hydrindane core skeleton.

Keywords: formal synthesis; natural products; picrotoxane sesquiterpenoids



(-)-Picrotoxinin

(+)methyl Picrotoxate

Organic Synthesis and Medicinal Chemistry (OM-P-037)

Palladium-mediated ortho C–H bond activation and arylation of 7-arylpyrazolo [1,5-a]pyridines applied in synthesis of novel 7,7′-di(2-biaryl)-3,3’-bipyrazolo [1,5-a]pyridine-based luminogens

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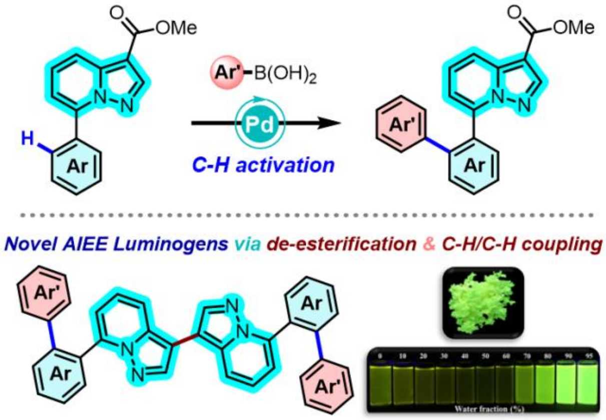
Pyrazolo[1,5-a]pyridines constitute an important class of fused nitrogen-containing heterocycles that exhibit a wide range of biological activities and optoelectronic properties. The introduction of aryl substituents at the 7-position of the pyrazolo[1,5-a]pyridine core further enhances their physicochemical properties, expanding their potential applications in material science and pharmaceutical development. In this work, a palladium-mediated ortho C–H bond activation and arylation of 7-arylpyrazolo[1,5-a]pyridine has been developed, enabling the synthesis of 7-(2-biaryl)-substituted pyrazolo[1,5-a]pyridine via both stoichiometric and catalytic approaches. In the stoichiometric reaction, pyrazolo[1,5-a]pyridine palladacycles featuring acetate and trifluoroacetate ligands were successfully isolated and characterized using X-ray crystallography. To gain deeper insights into the ortho C–H bond cleavage, parallel and intermolecular kinetic isotope effect studies were conducted, providing support for the proposed reaction mechanism. Finally, the developed methodology was applied to the synthesis of 7,7’-di(2-biaryl)-3,3’-bipyrazolo[1,5-a]pyridine-based luminogens, whose fundamental photophysical properties were measured, highlighting their aggregation-induced emission characteristics. Their fundamental photophysical properties, including UV-Vis absorption, photoluminescence (PL), and quantum yield (QY), were measured, showcasing unique luminescent characteristics. We believe this methodology offers chemists a facile route to construct analogous molecular skeletons and expand their applications across various fields [*Chem. Commun.* **2021**, *57*, 12281–12284; *J. Org. Chem.* **2022**, *87*, 9851–9863].

Keywords: palladium; C–H bond activation; pyrazolo[1,5-a]pyridine; palladacycles; AIE luminogens



Organic Synthesis and Medicinal Chemistry (OM-P-039)

Denitrogenative cyclization of benzothiatriazines to seven-membered sultams

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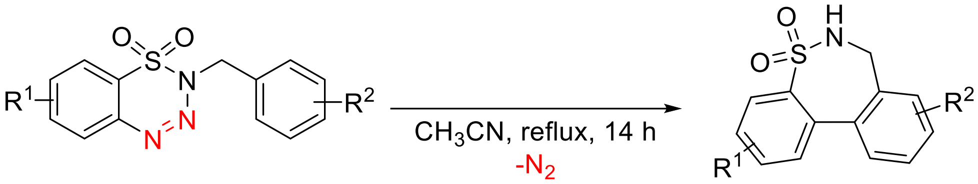
Sulfonamides are essential pharmacophores with broad applications in medicinal chemistry. Among them, cyclic sulfonamides, or sultams, are particularly significant as lactam mimics and are commonly found in bioactive compounds and pharmaceuticals. Due to their importance, various strategies have been developed to enable sultam synthesis. In this work, we report a transition metal-free approach for synthesizing 7-membered sultams via the denitrogenation of benzothiatriazenes, providing an efficient and practical method for accessing these valuable scaffolds.

Keywords: metal-free; cyclization; annulations; nitrogen compounds; substituents



✓ mild reaction conditions ✓ metal-free ✓ 26 examples, up to 88% yield

Organic Synthesis and Medicinal Chemistry (OM-P-040)

Oxidative scission of bicyclo[2.2.2]octenones via ketoxime fragmentation and Schmidt-type reactions

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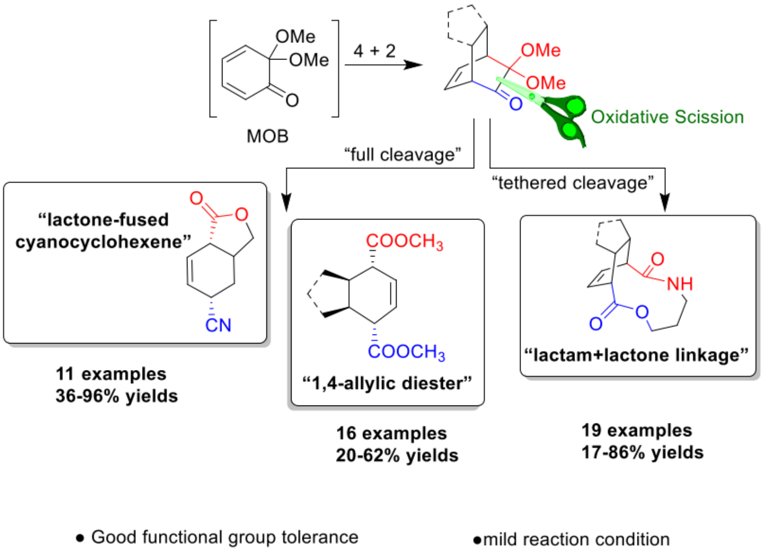
This study investigates the selective oxidative scission of bicyclo[2.2.2]octenones derived from masked o-benzoquinones (MOBs). Utilizing ketoxime fragmentation and Schmidt-type reactions, we successfully cleaved α-dimethoxy carbonyl groups, affording highly functionalized cyclohexene frameworks. This transformation highlights the expanding synthetic versatility of bicyclo[2.2.2]octenones in complex organic synthesis. The methodologies developed herein are expected to contribute to advancements in both organic and pharmaceutical chemistry.

Keywords: bond cleavage; oxidation reactions; rearrangement; ketoxime fragmentation; Schmidt-type reactions



Organic Synthesis and Medicinal Chemistry (OM-P-045)

Cyclopropanation of masked *o*-benzoquinones: A versatile route to tropolone derivatives

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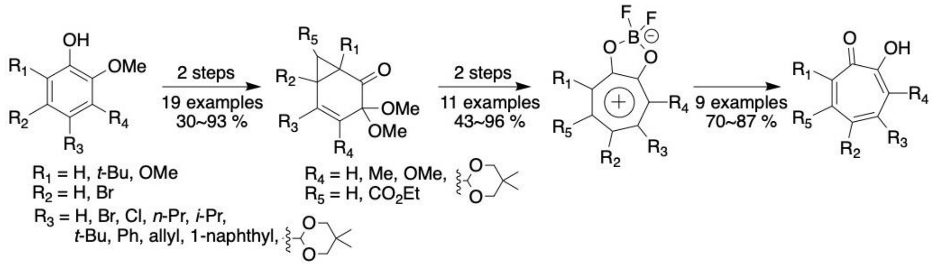
The Corey–Chaykovsky cyclopropanation of readily accessible masked *o*-benzoquinones (MOBs) has been explored to synthesize functionalized bicyclo[4.1.0]heptane derivatives with high regioselectivity. These bicyclic intermediates were subsequently transformed through a sequence involving hydrolysis, $BF_3 \cdot Et_2O$-mediated ring opening, and a final hydrolysis step to yield a variety of tropolone derivatives—a class of compounds with broad importance in synthetic, biological, and theoretical chemistry. By refining key steps within established cyclopropanation and ring-opening protocols, we have developed an improved synthetic route that allows access to a range of bicyclo[4.1.0]heptanes, tropolone difluorides, and tropolones from readily available MOB precursors. Our work emphasizes the generality and practical utility of this methodology.

Keywords: masked *o*-benzoquinone; bicyclo[4,1,0]heptane; tropolones



Organic Synthesis and Medicinal Chemistry (OM-P-046)

Rh-catalyzed C−H activation/C=C bond cleavage for functionalized aza-spiro *α*-retralones and benzoisoindoles

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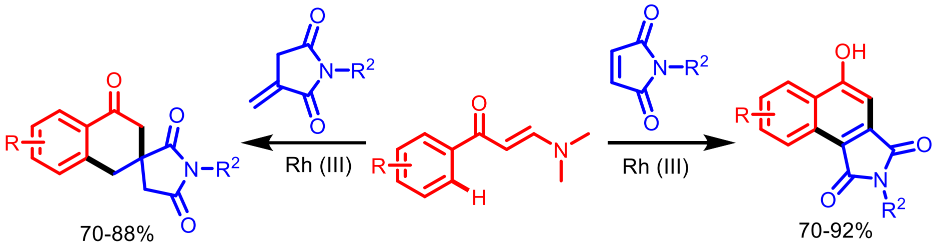
The *α*-tetralones and spiro *α*-tetralones are abundant moieties in naturally occurring and biologically active molecules. The benzo[*e*]isoindole scaffold is a structural framework that has been employed in the preparation of glycogen synthase kinase-3 (GSK-3) inhibitor, used to treat a variety of disorders, such as Alzheimer's disease, diabetes, colorectal cancer, and bipolar disorder. Therefore, we devised a new methodology for the synthesis of biologically interesting aza-spiro *α*-tetralones and benzo[*e*]isoindoles by Rh(III)-catalyzed C−H activation/ C=C bond cleavage of *β*-enaminones. This protocol provides a one-pot catalytic methodology for the synthesis of diversely functionalized aza-spiro *α*-tetralones and benzo[*e*]isoindoles in good yields, displaying a good substrate scope, outstanding functional group tolerance, and excellent regioselectivity under mild reaction conditions.

Keywords: Rh-catalyzed reaction; C−H activation/C=C bond cleavage; [4+2] annulation; *α*-tetralones; benzoisoindoles



Organic Synthesis and Medicinal Chemistry (OM-P-048)

One-pot synthesis of *O*-glycosyl propargylamine analogues

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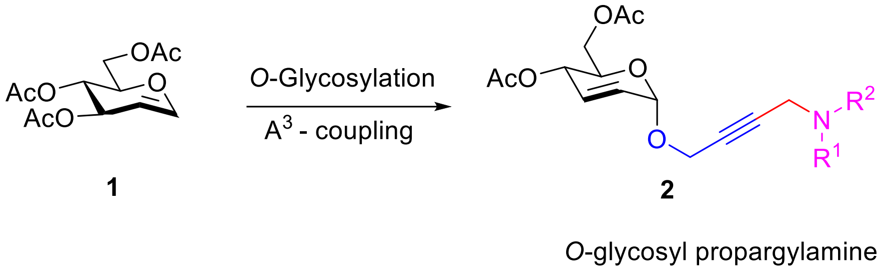
The synthesis of glycosides plays a crucial role in carbohydrate chemistry, enabling the attachment of diverse carbon chains to the sugar ring at the anomeric position. Glycosides exhibit a wide range of biological activities, including antiviral, antibacterial, antifungal, and anti-inflammatory properties. This study presents a straightforward one-pot, two-step approach for the synthesis of *O*-glycosyl propargylamines. In the first step, D-glucal reacts with propargyl alcohol to generate an *O*-propargyl glycoside. The second step involves a three-component A^3 coupling reaction with formaldehyde and various amines, yielding the desired O-glycosyl propargylamines in moderate to excellent yields (32–98%). To demonstrate the efficiency of this method, a total of 20 examples were synthesized and characterized.

Keywords: *O*-glycosyl propargylamine; glycosylation; A^3 coupling; one pot; D-glucal



Organic Synthesis and Medicinal Chemistry (OM-P-049)

Synthesis of 3-chalcogenide-indoles analogues

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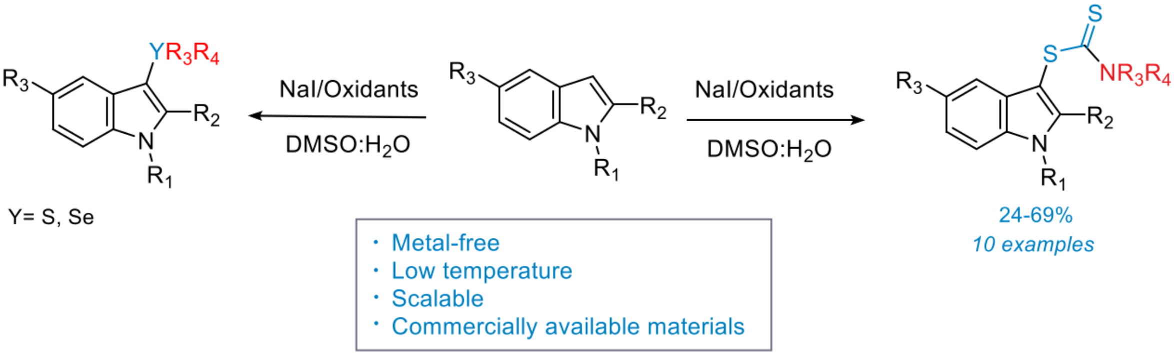
Chalcogenation, the process of introducing sulfur or selenium into the indole framework, has gained significant attention due to its relevance in medicinal and synthetic chemistry. Indoles are crucial heterocyclic scaffolds commonly found in bioactive natural products and pharmaceutical compounds. Among various indole derivatives, 3-sulfenylindoles have garnered increasing interest due to their remarkable biological and medicinal properties, including anti-inflammatory activity, inhibition of tubulin polymerization, HIV-inhibitory effects, and antiproliferative activity. In this study, we present an efficient method for C–S bond formation at the C3 position of indole using a range of iodine sources and oxidants. Notably, sodium iodide (NaI) as the iodine source facilitated the synthesis of 3-sulfenylindoles and new 3-dithiocarbamate analogues in good yields (24–69%). This approach offers an environmentally friendly, moisture-insensitive alternative that eliminates the need for metal catalysts.

Keywords: indole; 3-dithiocarbamate indoles; 3-sulfenylindoles; chalcogenation



- Metal-free
- Low temperature
- Scalable
- Commercially available materials

Organic Synthesis and Medicinal Chemistry (OM-P-050)

Photoswitchable BOAHY-BODIPY dyads as photosensitizers for photodynamic therapy

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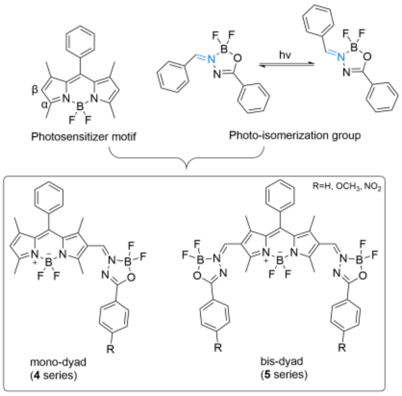
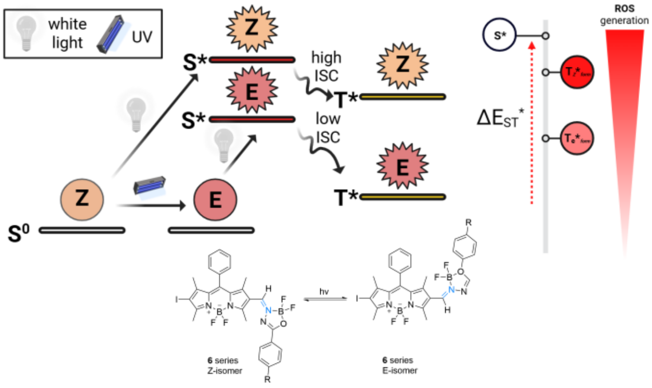
Photopharmacology, an innovative approach enabling precise temporal and spatial control of drug activity using light, includes photodynamic therapy (PDT), prodrug decaging, and photoisomerization-induced bioactivity. PDT utilizes photosensitizers (PSs) that, upon illumination, generate reactive oxygen species (ROS) to selectively induce cancer cell death. However, conventional PSs can damage healthy tissues due to lack of precise control.

To overcome this, we developed a novel photoswitchable PS based on a boron-acylhydrozone- boron-dipyrromethene (BOAHY-BODIPY) dyad system. By combining the strong photophysical properties of BODIPY with BOAHY's photoisomerization behavior, we synthesized mono- (4 series) and bis- (5 series) conjugates with efficient photoswitching and potent photocytotoxicity in vitro. Further iodinated derivatives (6 series) exhibited enhanced intersystem crossing and type-II ROS generation, attributed to reduced singlet–triplet energy gaps. This photoswitchable system enables initial therapeutic ROS activation under white light, while subsequent ultraviolet (UV) irradiation significantly deactivates residual PSs in normal cells (outside targeted regions), thus minimizing off-target effects. UV irradiation triggers Z-to-E isomerization, converting PSs into a less phototoxic form. Consequently, potential accidental sunlight exposure post-treatment poses minimal risk of off-target tissue damage, as these residual PSs remain inactive. This pioneering photoswitchable PDT platform thus represents a significant advancement toward safer and more selective cancer therapies.

Keywords: PDT; photosensitizer; BODIPY; photoisomerization





Organic Synthesis and Medicinal Chemistry (OM-P-051)

Enhanced Biginelli reaction via synergistic action of squaramide and TBAB ionic liquid

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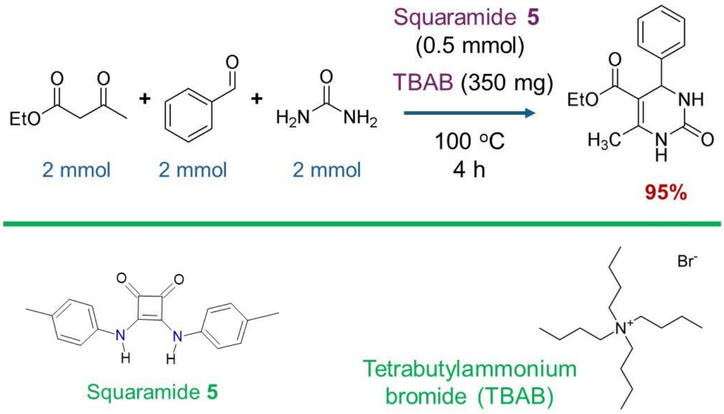
Multicomponent reactions (MCRs) have emerged as powerful tools in modern organic and medicinal chemistry for their efficiency, atom economy, and structural diversity. Among these, the Biginelli reaction—a one-pot, acid-catalyzed cyclocondensation of ethyl acetoacetate, benzaldehyde, and urea—remains a cornerstone method for synthesizing dihydropyrimidinones (DHPMs), valuable scaffolds in drug development. Traditionally, reactions were performed under reflux in ethanol with hydrochloric acid. In this study, we unveil a highly efficient alternative by leveraging the synergistic catalytic effect of squaramide derivatives and tetrabutylammonium bromide (TBAB), an ionic liquid, in the Biginelli reaction. A comparative screening of squaric acid and squaramides identified squaramide **5** as the most effective catalyst. Under optimized conditions—using TBAB as the solvent and squaramide **5** in catalytic amounts—the reaction proceeded smoothly to afford DHPM in an impressive 95% yield. In stark contrast, omitting squaramide **5** from the TBAB system resulted in a drastically lower yield (38%), and performing the reaction in ethanol with squaramide **5** gave only 34%. These findings underscore the remarkable synergy between squaramide **5** and TBAB, highlighting a potent, eco-friendly organocatalytic system for the Biginelli condensation and offering promising potential for broader synthetic applications.

Keywords: Biginelli; Squaramide; TBAB; Ionic liquid; dihydropyrimidinone



Organic Synthesis and Medicinal Chemistry (OM-P-053)

Sustainable peptide cyclization: A solvent-free anion-templated mechanochemical approach

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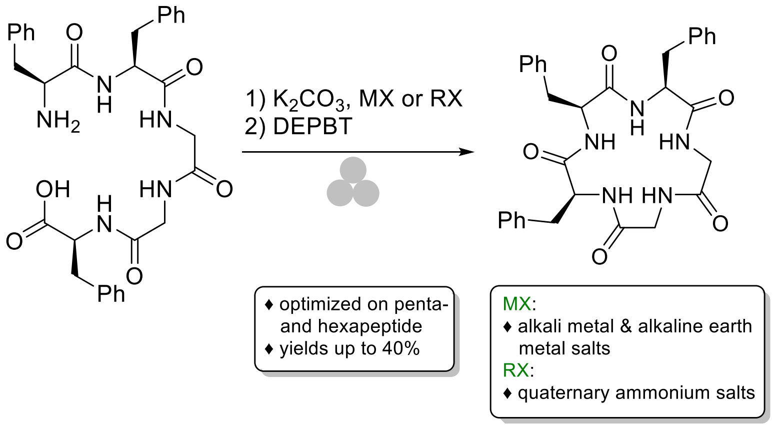
Peptide macrocyclization is a cornerstone of synthetic organic and medicinal chemistry due to the remarkable biological activity of cyclic peptides, making them ideal candidates for drug development. Traditional *head-to-tail* macrocyclization of corresponding linear peptides usually requires high dilution conditions in formamide solvents to avoid unwanted oligo- and polymerization reactions. The efficiency of cyclization, in some cases, is also dependent on the length of the peptide backbone and amino acid sequence.

As part of research in anion-templated peptide macrocyclization, we have developed a solvent-free macrocyclization to avoid the problems the solution-based approach suffers from. Linear precursors H-Phe-Phe-Gly-Gly-Phe-OH and H-Phe-Phe-Gly-Gly-Phe-Phe-OH were prepared using conventional methods and we utilized our cyclization strategy both in solution and mechanochemically. Linear peptides were cyclized by milling with potassium carbonate as a base, diethyl 4-oxo-1,2,3-benzotriazin-3(4*H*)-yl phosphate (DEPBT) as the coupling reagent and different salts as templating agents, particularly quaternary ammonium salts. This is, to our knowledge, the first time mechanochemical peptide macrocyclization has been achieved which provides a straightforward and green alternative in the field of cyclopeptide synthesis.

This project is funded by The European Union – NextGenerationEU project ToSiAn (Total synthesis of bioactive metabolites – From deep sea microorganisms to new class of antibiotics and synthetic methodologies, NPOO.C3.2.R2-I1.06.0043).

Keywords: ball-milling; cyclization; green chemistry; peptides



Organic Synthesis and Medicinal Chemistry (OM-P-054)

Design, synthesis and antimicrobial activity of 6-phenyl-4-azaindole derivatives

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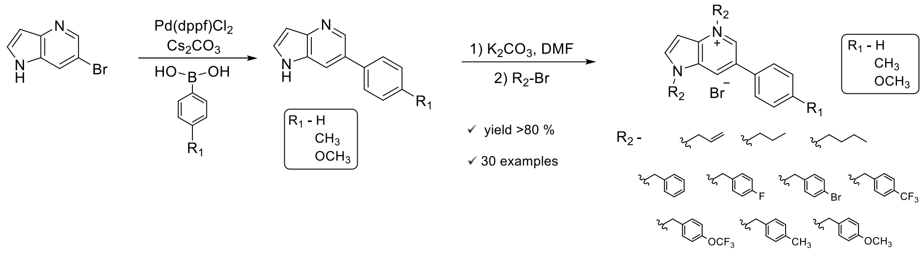
Heterocyclic compounds known as 4-azaindoles are structurally related to indoles, featuring a nitrogen atom instead of a carbon at the 4-position of the benzene ring. This structural modification often improves pharmacokinetic profiles such as solubility and metabolic stability. They have been investigated as core scaffolds in kinase inhibitors, antiviral agents, and central nervous system therapeutics. In this study, we designed and synthesized a series of 6-phenyl-4-azaindole derivatives featuring various substituents on the phenyl ring, starting from commercially available 6-bromo-4-azaindole via Suzuki coupling. The resulting compounds were further modified through alkylation of the pyrrole and pyridine nitrogen atoms using a range of alkyl and benzyl groups. The structures of all prepared compounds were determined by 1D and 2D ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy (NMR) and high-resolution mass spectrometry (HRMS). The antimicrobial potential of the compounds was evaluated against a panel of Gram-positive and Gram-negative bacteria, and their minimum inhibitory concentrations (MICs) were determined. All tested compounds exhibited potent inhibitory activity, demonstrating promising antimicrobial properties and potential for further development. This project is funded by The European Union – NextGenerationEU project ToSiAn (Total synthesis of bioactive metabolites – From deep sea microorganisms to new class of antibiotics and synthetic methodologies, NPOO.C3.2.R2-I1.06.0043).

Keywords: 4-azaindoles; Suzuki coupling; antimicrobial activity



✓ yield >80 %
✓ 30 examples

Organic Synthesis and Medicinal Chemistry (OM-P-056)

Synthetic study of emetine; Functionalization of the piperidine ring by oxidative vinylogous Mannich reaction

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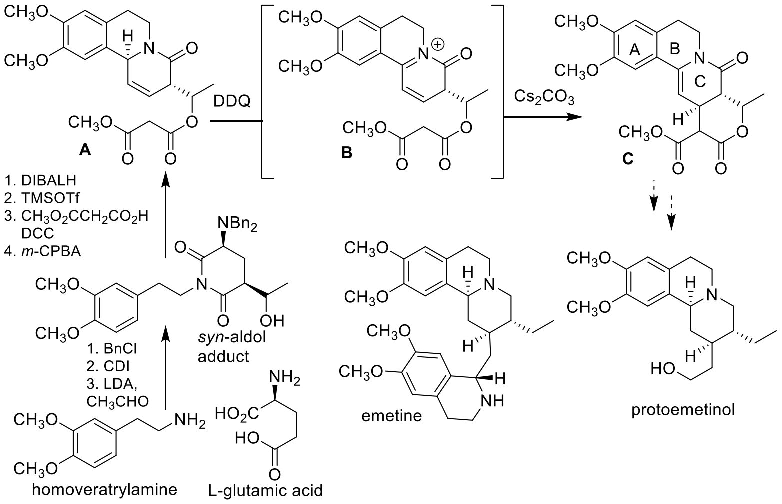
Benzoquinolizidine is an important structural feature found in many biological active alkaloids. Emetine is a cytotoxic benzoquinolizidine alkaloid found in the root of the *Psychotria ipecacuanha*. It has been used as anti-protozoal drug and exhibits emetic property. Our synthetic study of protoemetinol, the precursor of emetine led to benzoquinolizidinyl ethyl malonate ester **A.** We envision installation of malonate moiety on the piperidone **C** ring to be achieved by oxidative vinylogous Mannich reaction of unsaturated lactam **A** via *N*-acyliminium ion **B**. In this presentation, we discuss synthesis of precursor **A** from L-glutamic acid and the conditions that affect the oxidative vinylogous Mannich reaction. DDQ was used as oxidant while cesium carbonate was used as base to affect the diastereoselective formation of the lactone **C**. The lactone is the precursor for protoemetinol via decarboxylation and ester reduction. Synthesis of emetine from protoemetinol would be carried out using reported procedure.

Keywords: emetine; synthesis; vinylogous; Mannich reaction



Organic Synthesis and Medicinal Chemistry (OM-P-057)

Total synthesis of piperlongumine and its analogs from L-glutamic acid

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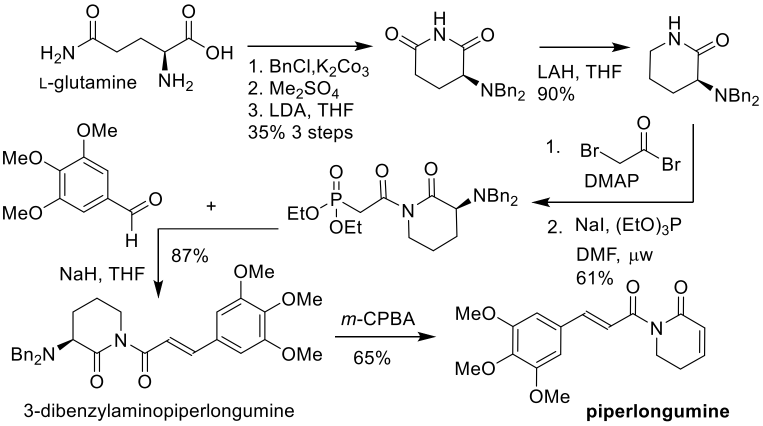
Piperlongumine is a cytotoxic alkaloid found in *Piper longum* (Deepli) which is used as spice and medicinal herb in Thailand and other countries in South and Southeast Asia. We have synthesized piperlongumine and its 3-dibenzylaminopiperlongumine analog from L-glutamic acid and 3,4,5-trimethoxycinamaldehyde. (3*S*)-Dibenzylaminoglutarimide was formed in 3 steps from L-glutamine via *N*-benzylation, methyl ester formation and cyclization in basic condition. Reduction of one of the glutarimide carbonyl with LAH gave 3-dibenzylamino-δ-lactam. *N*-Acylation of this compound with bromoacetyl bromide gave the bromoacetyl precursor which underwent HWE reaction with 3,4,5-trimethoxycinnamaldehyde. The product is 3-dibenzylaminopiperlongumine which was converted to piperlongumine by Cope elimination. In addition, the amino group will provide a variation point for further synthesis of other analogs of piperlongumine for evaluation of medicinal properties of the synthetic compounds in the future.

Keywords: piperlongumine; analogs; synthesis



Organic Synthesis and Medicinal Chemistry (OM-P-060)

Planar-chiral skewed DPPF derivatives: Design, synthesis, and application of novel C_2-symmetric chiral bisphosphine ligands

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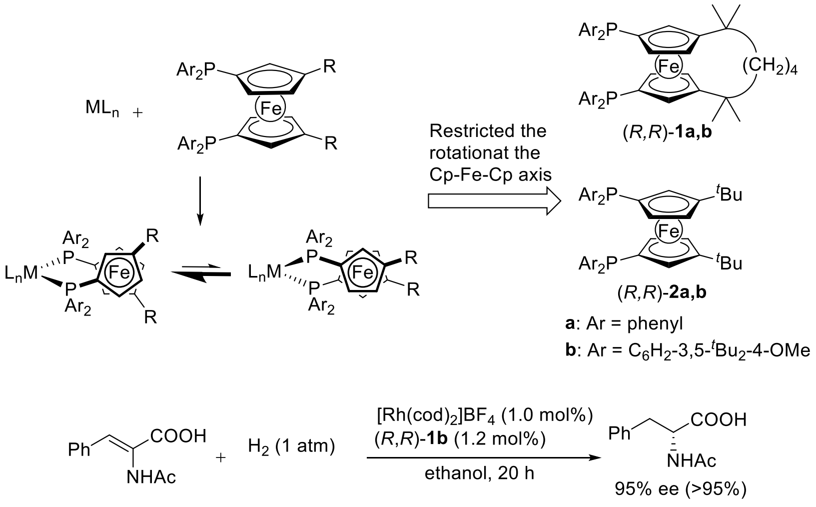
DPPF (1,1'-bis(diphenylphosphino)ferrocene) is a bidentate phosphine ligand with unique steric and electronic properties and have been applied in various transition-metal catalyses as a useful ancillary ligand. Upon the chelate coordination to a metal center, DPPF takes a skewed chiral (but racemic) conformation as shown in Figure (top left). We envisioned that if the skewed conformation could be frozen somehow, DPPF could be utilized as a novel chiral phosphine ligand. Our strategies to realize this idea is introduction of proper substituents, such as a bridging component between the two Cp-rings or bulky substituents sterically interacting with each other, in DPPF at the positions remote from the diphenylphosphino-substituents, which restricted the rotation at the Cp-Fe-Cp axis (Figure, top left).

Based on the design concept mentioned above, a series of planar-chiral DPPF derivatives **1a**,**b** and **2a**,**b** were prepared in enantiomerically pure forms (Figure, top right). These novel chiral ligands were applied in the rhodium-catalyzed asymmetric hydrogenation and showed promising results of up to 95% ee (Figure, bottom). Details of these results will be presented at the congress.

Keywords: ferrocene; planar-chiral; phosphine; hydrogenation; asymmetric



Polymers and Bio-based Materials (PC-P-001)

Synthesis of 3,4-disubstituted thiophene-based π-conjugated polymers *via* nonstoichiometric direct arylation polycondensation

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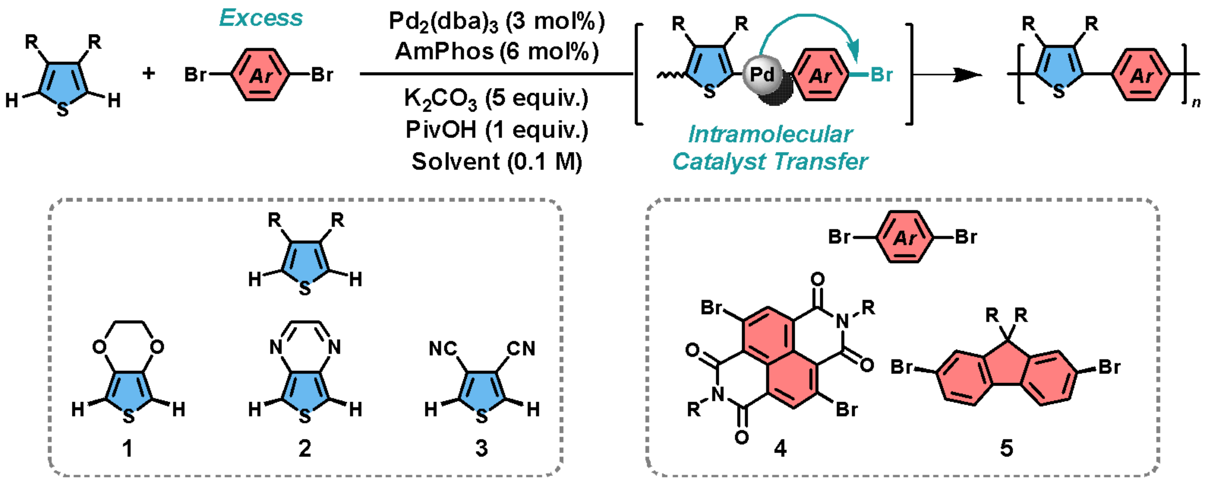
π-Conjugated polymers offer a wide range of potential applications, including organic light-emitting diodes, organic field-effect transistors, organic electrochemical transistors, organic solar cells, organic thermoelectric devices, photocatalysts, sensors, supercapacitors, and memory devices. To obtain high-molecular-weight π-conjugated polymers in conventional AA+BB-type polycondensation in a single-phased solution, stoichiometry control of monomer ratios is essential. Conversely, the intramolecular catalyst transfer system enables to synthesize high-molecular-weight π-conjugated polymers *via* Suzuki–Miyaura, Migita–Kosugi–Stille cross-coupling or direct arylation polycondensation (DArP) reactions under nonstoichiometric conditions as previously reported. [*Polym. Chem.* **2025**, *16*, 11–26] However, these reactions have challenges related to high costs and significant environmental impact due to the use of organometallic reagents such as boron, tin, or silver elements.

In this study, we found that the palladium-catalyzed DArP, that does not require other transition metal components, efficiently proceeded even under nonstoichiometric conditions for the first time. For instance, DArP between 3,4-ethylenedioxythiophene monomer (**1**) and 1–3-fold excess of naphthalene-diimide-based dibromo-monomer (**4**) afforded high-molecular-weight π-conjugated polymers with the number-average molecular weight of 13,000–17,000. In addition, thieno[3,4-*b*]pyrazine (**2**) and 3,4-dicyanothiophene monomer (**3**) and fluorene-based dibromo monomer (**5**) were also applicable to this polycondensation system.

Keywords: π-conjugated polymers; direct arylation polymerization; nonstoichiometric polycondensation; intramolecular catalyst transfer; environmentally friendly



Polymers and Bio-based Materials (PC-P-007)

Effect of surface bentonite and surface modified bentonite on the moisture absorption of starch-based composite foams

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This study aimed to investigate the effect of bentonite and surface-modified bentonite on the moisture absorption and structural properties of thermoplastic starch-based foams. Bentonite, a naturally occurring clay mineral, was selected due to its abundance and high ion-exchange capacity. To increase its hydrophobicity and compatibility with starch, soy lecithin, which is amphiphilic, non-toxic, and biodegradable, was used for surface modification. The modification process involved dispersing bentonite in an ethanolic soy lecithin solution followed by controlled drying. FTIR spectra confirmed successful modification through the appearance of a characteristic carbonyl (C=O) band at 1739 cm^{-1}. Thermogravimetric analysis further supported the modification by revealing higher decomposition temperatures and increased residual weight at 700°C for the treated bentonite. The incorporation of both untreated and modified bentonite enhanced starch-filler interactions, resulting in increased foam density and improved structural integrity. Notably, foams containing modified bentonite showed significantly lower moisture absorption, indicating enhanced hydrophobicity. This study highlights the potential of surface-modified bentonite as a green reinforcing agent in biodegradable foams, offering promising applications in sustainable packaging and bio-based materials.

Keywords: bentonite; soy lecithin; thermoplastic starch; moisture absorption

Polymers and Bio-based Materials (PC-P-009)

Control of induced chirality in supramolecular gel-cyanine dye complexes by multivalent anions

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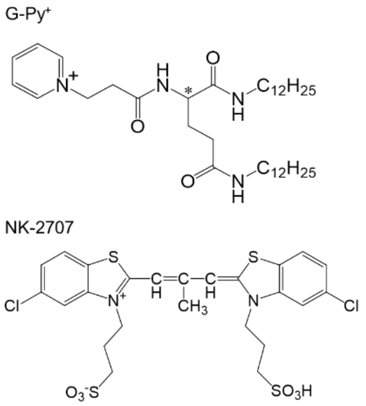
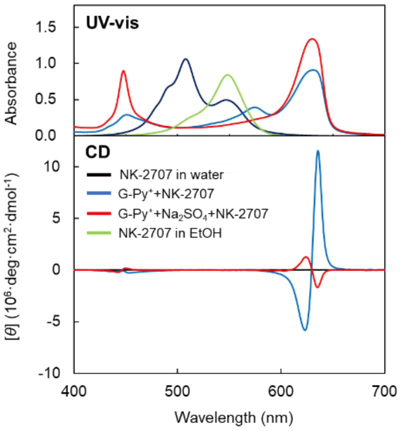
Supramolecular assemblies with ordered structures can express and amplify functions not achievable by individual molecules, making them promising for the development of novel optical materials. In this study, we investigate the effect of multivalent anions on the induced chirality of anionic cyanine dyes bound to nanofibrous supramolecular gel formed from cationic L-glutamide derivative (G-Py$^+$, see Figure). UV-vis spectra showed that the cyanine dye, NK-2707 (see Figure) existed in monomeric (550 nm) and H-aggregate (505 nm) states in aqueous solution. When NK-2707 was added to aqueous solution of self-assembled G-Py$^+$ (NK-2707 : G-Py$^+$ = 1:40 (mol/mol)), adsorption peaks shifted to 450, 570 and 630 nm. Remarkably large circular dichroism (CD) signals were observed at 623 nm (negative) and 635 nm (positive), and small CD signals were observed around 447 and 454 nm. These results indicated that NK-2707 formed R-chiral H-aggregate and S-chiral J-aggregate on the G-Py$^+$ self-assemblies. Interestingly, the addition of Na_2SO_4 resulted in sign reversals of the CD signals of H- and J-aggregates, although no sign reversal was observed by addition of NaCl or Na_2HPO_4. These results indicated that SO_4^{2-} significantly influence on the chiral microenvironment of G-Py$^+$ self-assemblies.

Keywords: self-assembly; supramolecular gel; induced chirality; anionic cyanine dye; glutamide derivative





Polymers and Bio-based Materials (PC-P-010)

Control of circular polarization properties of chiral supramolecular gels via complexation with achiral organic ligands

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Supramolecular metal complexes exhibit excellent optical, electronic, and magnetic properties, making them promising for materials in various applications. We have reported the induced chirality in chromophores bound to chiral supramolecular gels formed from glutamide-derivatives, and its control by the stimuli such as temperature, and salt. For instance, the glutamide-derived supramolecular gels with organic ligands such as isoquinoline, porphyrin, and terpyridine (G-tpy) could be controlled by the addition of metal ions. In this study, we demonstrate the modulation of circular dichroism (CD) and circularly polarized luminescence (CPL) signals of G-tpy complexed with metal ions (G-tpy(M)) by the addition of achiral ligands as guests. CD and CPL signals were negligible in self-assembled G-tpy alone, but were significantly increased by addition of metal ion such as Zn^{2+} (G-tpy(Zn)) and Cd^{2+} (G-tpy(Cd)). Addition of the achiral ligands 2,2':6',2"-terpyridine to G-tpy(M) resulted in a significant change in CD signal and sign reversal of CPL signal with a slight wavelength shift (shown in Figure). The observed chirality modulations are probably due to the changes in the coordination geometry of the complex, electronic state of metal ion, and steric effect of 2,2':6',2"-terpyridine on orientation structure of G-tpy.

Keywords: chiral self-assembly; circularly polarized luminescence (CPL); metal coordination; terpyridine; chirality inversion

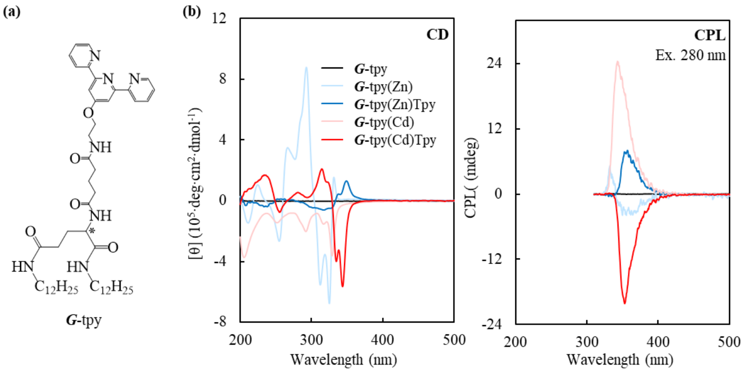

Fig. 1 (a) Chemical structure of ***G***-tpy. (b) CD and CPL spectra of ***G***-tpy, G-tpy(Zn), ***G***-tpy(Zn)Tpy, ***G***-tpy(Cd), ***G***-tpy(Cd)Tpy in cyclohexane-ethanol (9 : 1) solution at 10 ° C.[***G***-tpy] = [Metal ions] = [Tpy] = 0.25 mM

Polymers and Bio-based Materials (PC-P-012)

Chirality induction in polycyclic aromatic polymer thin films on helical nanosilica

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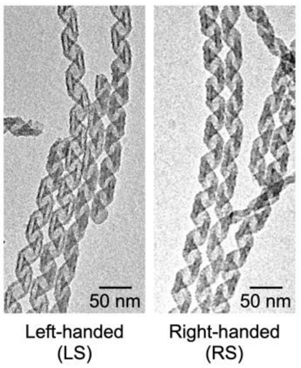
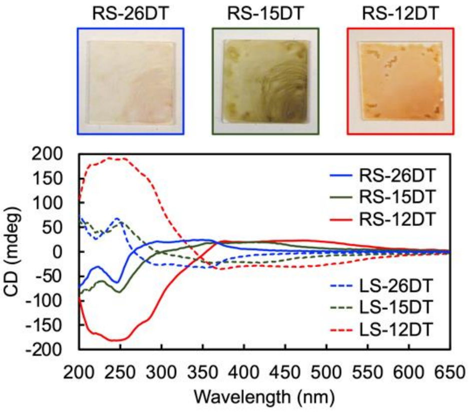
Circularly polarized materials are expected to be applied in next-generation optical technologies such as information, security and sensors. We recently reported the preparation of spherical polycyclic aromatic polymer particles using a one-pot process in which a solution of phenolic compounds such as 1,5-dihydroxynaphthalene (15D) was stirred with 1,3,5-trimethyl-1,3,5-triazinane (T) as a crosslinker. Polymer particles exhibit unique functions, for instance, selective near-infrared light reflection and fluorescence solvatochromism, and are expected to be applied as novel functional optical materials. In this study, we describe the preparation of wavelength-selective circular polarizing hybrid films by coating polycyclic aromatic polymers onto helical nanosilica. The films were prepared by drop-casting of 15D and T mixed solution with right- and left-handed helical nanosilica (RS, LS) on quartz glass. The solution was dried under ambient atmosphere, and heating at 100 °C for 3 hours (RS-15DT, LS-15DT). Mirror circular dichroism (CD) signals were observed in RS-15DT and LS-15DT around 420 nm, corresponding to the absorption of the 15DT polymer. When 1,2-dihydroxynaphthalene (12D) and 2,6-dihydroxynaphthalene (26D) were used instead of 15D, similar symmetric CD signals were observed around 475 nm and 350 nm. The wavelength of the CD signal can be controlled by preparing hybrid films with different phenolic compounds.

Keywords: circular dichroism; circularly polarized luminescence; naphthoxazine polymer

TEM images of helical nanosilica





CD spectra of hybrid films

Polymers and Bio-based Materials (PC-P-018)

Synthesis of diketopyrrolopyrrole-based semiconducting polymers with urea and 1,2,3-triazole groups on their side chains

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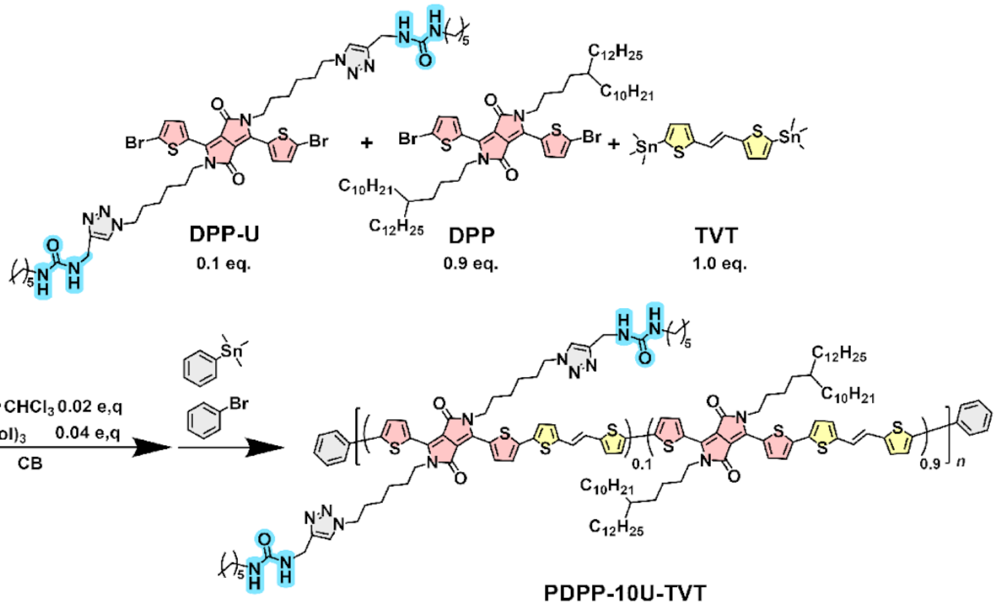
In recent years, electronic devices have become lighter and more flexible, and the application to wearable devices has currently been demanded for medical and healthcare fields. The thermal stability of semiconducting polymers is one of the important factors aiming at fabrication of various organic electronic devices.

In this study, the facile synthesis of a thermally-stable diketopyrrolopyrrole (DPP)-based semiconducting polymer with urea and 1,2,3-triazole groups in its side chain, **PDPP-10U-TVT**, is presented. According to **Scheme 1**, statistical ternary copolymerization was performed based on Migita-Kosugi-Stille coupling reaction between **DPP-U** (0.1 eq.), **DPP** (0.1 eq.), and **TVT** (1.0 eq.) in the presence of $Pd_2(dba)_3 \cdot CHCl_3$ in chlorobenzene, followed by end-capping reaction with trimethyl(phenyl)stannane and bromobenzene. As a result, **PDPP-10U-TVT** (containing 10 mol% urea-based side chains) with the number average molar-mass (M_n) of 11,000 g/mol and molar-mass distribution (M_w/M_n) of 1.74 was obtained. In the FT-IR spectrum of **PDPP-10U-TVT**, an absorption peak around 3400 cm^{-1} was observed, which was attributed to the hydrogen-bonded urea groups. Interestingly, the presence of urea units improved 5% weight-loss temperature up to 396 °C as determined by TGA, which is much higher than the reference DPP-based semiconducting polymer without urea units by 80 °C. This is probably derived from the effect of 3D network structures of hydrogen bonds between polymers.

Keywords: π conjugated polymer; semiconductor polymer; urea; hydrogen bonds



Polymers and Bio-based Materials (PC-P-021)

Ecotoxicological assessment of polypropylene microplastics of different sizes on some marine organisms

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Plastic pollution poses a serious threat to human health, ecosystems and the environment. In particular, the negative effects of microplastics (MPs) have become the focus of recent research interest. This study aimed to explore the effect of recyclable polypropylene (PP) derived from commercial disposable on four marine crustaceans. The acute lethal responses were investigated in: a copepoda *Tigriopus fulvus*, two amphipods *Corophium insidiosum* and *Gammarus aequicauda* and an isopod *Cymodoce truncata.* PP leachates and PP microplastics (MPs) of two different sizes (from 20 to 38 µm and from 38 to 200 µm) were evaluated in acute toxicity tests during the exposure period of 96h. The responses of all tested crustaceans did not evidence any significant effect of acute toxicity to leachates, even at the 100% concentration.

PP MPs of 20-38 µm size elicited high toxicity to *G. aequicauda*, *C. truncata* juveniles and *T. fulvus* nauplii. While no acute response was observed for *C. insidiosum* also at the highest concentration tested (100 mg/L). No effects were observed for PP MPs of 38-200 µm size.
In conclusion, PP MPs have the potential to be toxic to marine crustaceans, with the smaller microplastics proving to be potentially more dangerous.

Keywords: acute toxicity test; polypropylene; microplastics; leachates; marine crustaceans

Synthesis of a novel star-shaped poly(3-hexylthiophene) with a hydroxyl group at the end of each arm polymer chain

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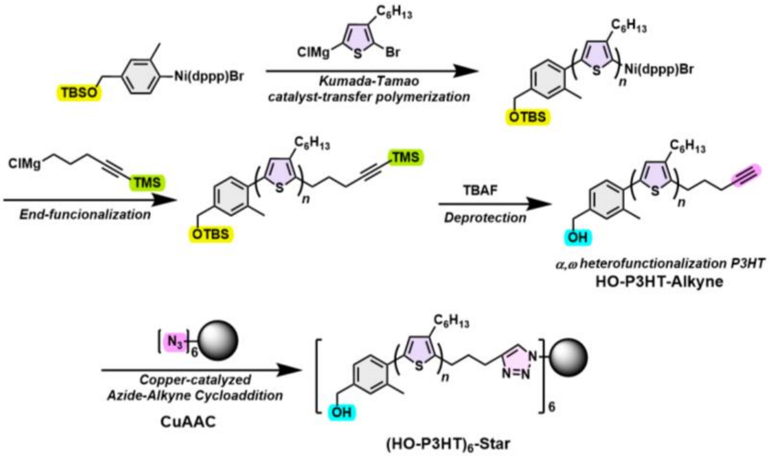
Semiconductor polymers are promising for stretchable electronic devices due to their excellent stress relaxation. However, further molecular design is needed to achieve long-term durability, especially in three-dimentional stress relaxation and self-healing. In this study, we focus on star-branched polymers with arms extending in three dimensions.Indeed, a novel six-armed star-branched poly(3-hexylthiophene) with a hydroxyl group at the end of each arm segment (**(HO-P3HT)$_6$-Star**) was first synthesized.

(HO-P3HT)$_6$-Star was synthesized *via* a copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction between α,ω-heterofunctionalized P3HT with a hydroxyl and alkyne group (**HO-P3HT-Alkyne**) and a core compound with six azide groups (**(N$_3$)$_6$-core**) (**Scheme 1**). The SEC curve of the resulting polymer mixture showed the peak shift to the high molecular weight side compared to that of arm polymer, **HO-P3HT-Alkyne**, suggesting the progress of the polymer linking reaction. The FT-IR spectrum of **(HO-P3HT)$_6$-Star** showed the complete disappearance of the absorption peak around 2100 cm^{-1} assignable to the azide groups introduced in the core compound, indicating high polymer linking efficiency.

Hydroxyl groups are expected to improve the adhesion and self-healing properties of the polymer, and can be converted to azide or alkyne groups, further multifunctionalizing the corona structures of star-branched polymers with various functional groups/polymers via the CuAAC reaction.

Keywords: π-conjugated polymers; poly(3-hexylthiophene); star polymer; branched polymer; hydroxyl group



Polymers and Bio-based Materials (PC-P-029)

Cellular responses of MC3T3-E1 on peptide-functionalized chitosan

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Chitosan, a biocompatible biomaterial, has been widely explored for bone regeneration applications, with chemical modifications enhancing its osteogenic properties. In this study, extracellular matrix (ECM)-derived peptides including RGD (RGD) and Ten2 (VFDNFVLK), derived from canonical ECM proteins, fibronectin and tenascin C, respectively, were used. These thiol-tagged peptides were covalently conjugated to chitosan via N-(m-maleimidobenzoyloxy)succinimide (MBS), resulting in maleimide-conjugated chitosan (MB-chitosan, control), as well as peptide-conjugated chitosan variants, including RGD-chitosan and Ten2-chitosan. This work aimed to investigate how specific functional peptide sequences influence biological responses at various levels, including cell morphology, adhesion, and mineralization. The results revealed that MB-chitosan, RGD-chitosan, and Ten2-chitosan effectively facilitated cell adhesion, with adhesion percentage of 100, 122 ±14, and 117 ±18, respectively. Moreover, morphological changes, including cell spreading and the formation of well-defined actin filament structures, were observed during initial interactions under serum-free conditions. Notably, Ten2-chitosan significantly enhanced mineralization over a 21-day culture period, as indicated by a higher normalized calcium content (4.04 ±0.60 ng/ng total protein) compared to the mineralization control polystyrene (2.18 ±0.10 ng/ng total protein). Overall, improved cell adhesion and mineralization are indicative of osteoblast differentiation, implying the potential of the biomaterials to support bone regeneration.

Keywords: chitosan; peptide; surface conjugation; osteoblast

Polymers and Bio-based Materials (PC-P-030)

Acrylic polymer-based composites designed for radiative passive cooling applications

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Amid rising global temperatures and increasing energy consumption, radiative passive cooling paints have emerged as a sustainable and energy-efficient solution for various applications. These paints reflect sunlight while simultaneously allowing thermal radiation to be emitted into outer space, effectively reducing the surface's temperature without needing an external source. This study presents the development of radiative cooling paints based on thermoplastic-based composites from polymethyl methacrylate (PMMA) as the polymeric binder, commercial barium sulfate ($BaSO_4$) as the pigment, and titanium dioxide (TiO_2) as a secondary inorganic filler. These composites were formulated in various weight ratios, (30:60:10), (30:55:15), and (30:50:20), respectively. These ratios are critical in assessing the influence of different compositions on the optical performance, thermal properties, surface morphology, and crystallographic structure. UV–Vis–NIR spectrophotometry results showed that all PMMA-based composites exhibited significantly higher average reflectivity compared to pristine PMMA over the entire wavelength range (500–2500 nm). Furthermore, a notable decline in the average reflectance as the amount of TiO_2 increases was observed, which can be attributed to intrinsic absorption properties and the agglomeration of its particles at higher concentrations, as evidenced by SEM images. Therefore, a surface with a high solar reflectivity has a higher tendency to enhance passive cooling effectiveness.

Keywords: radiative cooling; atmospheric transparency window; thermal radiation; thermoplastics; reflective filler

Polymers and Bio-based Materials (PC-P-031)

Biodegradable plastic production using a novel methanotroph

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Methane is a potent greenhouse gas with a global warming potential 84 times greater than that of carbon dioxide, posing a significant threat to the stability of global ecosystems. On the other hand, it serves as a promising feedstock for biological conversion for the production of environmentally friendly, value-added products. In this study, we isolated a novel methanotroph, *Methylocystis* sp. KHU, from sewage sludge. Whole-genome analysis revealed that this strain possesses key genes required for the biosynthesis of polyhydroxybutyrate (PHB), a biodegradable plastic. Cultivation conditions were optimized to enhance PHB accumulation, and the strain was found to produce PHB, more than 60% of its dry weight, when it was grown on methane. GSM is applied for quantitative analysis of PHB production. These findings suggest that *Methylocystis* sp. KHU is a promising and eco-friendly microbial platform for converting methane emissions into biodegradable plastics, thereby contributing to climate change mitigation and resource circularity.

Keywords: methane; methanotroph; PHB; biodegradable plastics; *Methylocystis*

Physical and Theoretical Chemistry (PT-P-005)

Computational study of glyphosate adsorption on coordinatively unsaturated metal-organic frameworks $M_3(btc)_2$

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Adsorption is a key strategy for glyphosate removal, playing a crucial role in mitigating its harmful effects. In this work, we investigate glyphosate adsorption on metal–organic frameworks $M_3(btc)_2$ (M = Cr, Mn, Fe, Co, Ni, Cu, and Zn) using density functional theory (DFT) calculations with the M06-L functional. The most stable adsorption configuration features an interaction between the phosphoryl (P=O) group and the metal site of $M_3(btc)_2$. $Ni_3(btc)_2$ provides the highest adsorption free energy (–29.1 kcal/mol) as compared to ones of other MOFs. This result corresponds to its highest ordered Lewis acidity calculated by ammonia adsorption. A strong linear correlation between glyphosate and ammonia adsorption energies is observed, implying that the Lewis acidity of the MOF plays a significant role in the glyphosate adsorption process. Moreover, as the temperature increases, the equilibrium constants decrease for all adsorption systems. $Ni_3(BTC)_2$ exhibits the highest adsorption equilibrium constant across all the studied temperature series, which aligns with its adsorption energy. The findings in this work would help to understand the structure-property relationships for MOFs and are beneficial to discover a prospective material for adsorption and separation of organophosphate pesticides.

Keywords: glyphosate; adsorption; metal–organic frameworks; DFT

Physical and Theoretical Chemistry (PT-P-006)

Effect of the Lewis acidity of MFI zeolite nanosheets on glucose adsorption and isomerization to fructose: A DFT study

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The glucose adsorption and isomerization to fructose over Lewis acidic MFI zeolite nanosheets (MFI-NS) have been investigated by means of density functional calculations. The glucose adsorbs on the zeolite via its hydroxyl group at the active site, involving both Lewis acid–base and hydrogen–bonding interactions. The glucose adsorption energies on Sn-MFI-NS, Zr-MFI-NS, and Ge-MFI-NS are −39.3, −45.6 and –31.5 kcal/mol, respectively. The higher adsorption energy observed for Zr-MFI-NS can be attributed to the stronger Lewis acidity of its Zr site compared with the Sn and Ge sites, as evidenced by ammonia adsorption. A seven-step mechanism is proposed for the glucose isomerization reaction involving (1) the deprotonation of the glucose hydroxyl group, (2) ring opening via protonation of the oxygen atom in the six-membered ring, (3) the hydroxyl group deprotonation of the ring-opening adduct, (4) aldose–ketose isomerization via a hydride shift, (5) the deprotonation of the ketose hydroxyl group, (6) a ring-closure reaction yielding anionic fructofuranose, and (7) the protonation of the terminal oxygen anionic moiety to generate cyclic fructose. The overall activation barriers are 18.0, 16.2, and 34.8 kcal/mol for Sn-MFI-NS, Zr-MFI-NS, and Ge-MFI-NS, respectively. Hence, the catalytic activity follows the order Zr-MFI-NS > Sn-MFI-NS > Ge-MFI-NS.

Keywords: glucose; isomerization; lewis acidic zeolite; nanosheet; DFT

Physical and Theoretical Chemistry (PT-P-007)

Inverse design of organic semiconductor materials based on polycyclic aromatic hydrocarbons using artificial intelligence

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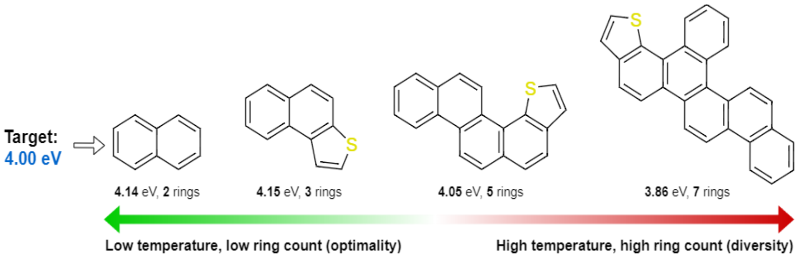
We present an artificial intelligence-driven approach for the inverse design of organic semiconductor materials based on polycyclic aromatic hydrocarbons (PAHs). Inverse design is a computational approach in materials discovery that flips the traditional workflow in computer-aided design where properties are predicted from known structures. Inverse design instead aims to design materials that obtain desired preset properties. It is, however, complex due to the non-uniqueness and nonlinear property-to-structure relationships. The effectiveness of this approach is demonstrated through the design of PAHs with specific band gaps, a key property for organic semiconductors such as organic light-emitting diodes. Our method generates PAH structures with band gaps ranging from 1.36 eV to 4.30 eV with an error of 0.15 eV within DFT uncertainty. To accomplish this, we employ goal-conditioned reinforcement learning with chemical domain knowledge. By incorporating the target property in the input, our model is explicitly aware of design goals. For chemical accessibility, our model includes a constraint minimizing the number of rings that favors simpler PAH designs. By balancing optimization and structural diversity, our pipeline overcomes key inverse design challenges while having a high degree of control, allowing prioritization of the best-performing solutions or a diverse set of candidates.

Keywords: inverse design; polycyclic aromatic hydrocarbon; reinforcement learning



Physical and Theoretical Chemistry (PT-P-008)

Computational insights into sulfonamide-modified cannabinoids as selective COX-2 inhibitors: Binding affinity and drug-like properties

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Cyclooxygenase (COX) is a key enzyme involved in inflammation and a major target for selective inhibition to reduce the adverse effects of nonsteroidal anti-inflammatory drugs (NSAIDs). This study employs a computational approach to evaluate the binding affinity and selectivity of sulfonamide-modified cannabinoids as potential COX-2 inhibitors. We applied semiempirical quantum mechanical (SQM) methods, particularly GFN2-xTB, to refine docked poses and predict binding free energies in implicit solvation ($\Delta G_{bind,solv}$). Within a fully relaxed COX-2 truncated pocket, noncovalent interactions of sulfonamide-modified cannabinoids contribute to $\Delta G_{bind,solv}$ values ranging from −35 to −64 kcal/mol, of which 27% to 49% is attributed to the sulfonamide group. These values indicate stronger binding than celecoxib ($\Delta G_{bind,solv} = -32.02$ kcal/mol), a known COX-2 selective NSAID. Additionally, drug-like properties and oral bioavailability predictions suggest favorable pharmacokinetics for these analogs. The findings highlight the potential of sulfonamide-modified cannabinoids as promising COX-2-selective inhibitors, providing valuable insights for the rational design of novel anti-inflammatory agents.

Keywords: NSAIDs; COX-2 inhibitors; sulfonamide cannabinoids; molecular docking; semiempirical quantum mechanics

Physical and Theoretical Chemistry (PT-P-009)

Iridium complexes as a photocatalyst: A triplet-singlet energy investigation

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Diazirine-based photoaffinity probes have been developed for proximity labeling. However, the directly activated diazirine requires ultraviolet (UV) light to function. To activate diazirine using visible light, a compound, which has triplet-singlet energy difference equal to or higher than 60 kcal/mol can be used as a photocatalyst for this process. One of the candidate compounds is $[Ir(dFCF_3ppy)_2(dtbbpy)^+]$, which has triplet-singlet state energy equal to 60 kcal/mol. This complex can be photoexcited using blue light and can then transfer energy to diazirine to generate carbene via the Dexter energy transfer mechanism. Due to its complex geometry, we explore the possibility of using simpler photocatalytic complex based on $[Ir(ppy)_3]$ for proximity labeling. However, the triplet-singlet state energy of $[Ir(ppy)_3]$ is known to be 55 kcal/mol, which is not enough to activate diazirine. In this work, we modify $[Ir(ppy)_3]$ and assess the triplet-singlet state energy of these complexes obtained using time-dependent density functional theory (TDDFT) with various functionals: B3LYP, M06-2X, CAM-B3LYP, wB97X, Pw6B95, PBEh, and B97 under the DCOSMO-RS solvation model. The results indicate that the solvation effect plays an important role, and TD-DFT tends to overestimate the triplet-singlet state energy in comparison with the experiment.

Keywords: TD-DFT; triplet state energy; $[Ir(ppy)_3]$; photocatalyst

Physical and Theoretical Chemistry (PT-P-010)

Crown ether design for lithium extraction: A quantum chemical study

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Lithium-ion batteries (LIBs) are increasingly utilized in modern automobiles. The demand for lithium-ion batteries is growing annually, raising concerns regarding potential lithium resource depletion. This necessitates the development of optimized protocols for lithium metal recycling from spent lithium-ion batteries. We propose a lithium extraction process based on the design of novel crown-ether-based compounds. To predict the lithium extraction performance of these compounds, quantum chemical calculations using the CREST and CENSO protocols were performed to obtain bound and unbound structures, as well as binding free energies. Our calculations reveal that certain compounds adopt a sandwich structure, with the lithium ion positioned above the bowl-shaped structure of the modified crown ether. The calculated binding free energies, ranging from 30.77 to 82.45 kcal/mol, support this structural observation and indicate a weak binding affinity between lithium and the compounds. Notably, these values are positive and consistent with those reported in the literature for similar compounds.

Keywords: crown ether; lithium; binding free energy; thermodynamic cycle

Physical and Theoretical Chemistry (PT-P-011)

Exploring 2D NiPS as a high-performance thermoelectric materials: First-principles calculations

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Achieving high-efficiency thermoelectric energy conversion requires materials with optimized electronic transport and suppressed thermal conductivity. In this work, we predict two novel Monolayer NiPS compounds and systematically assess their thermoelectric potential using first-principles calculations. Stability analyses, including cohesive and formation energy, phonon dispersion, and ab initio molecular dynamics simulations, confirm their structural robustness. Notably, a highly symmetric NiPS phase exhibits exceptional thermoelectric properties, with a figure of merit (ZT) surpassing 2 at temperatures exceeding 1000 K for both n-type and p-type conduction. These results position NiPS as a highly promising candidate for high-temperature thermoelectric applications, offering a rare balance between structural stability and enhanced transport properties.

Keywords: NiPS; thermoelectric material; density functional theory; two-dimensional mateiral

Catalytic Systems for Contemporary Challenges (S2-P-005)

Rational design of Cu^+ active species incorporated in hierarchical silicalite-1 via the electrochemical-assisted method for ethanol dehydrogenation

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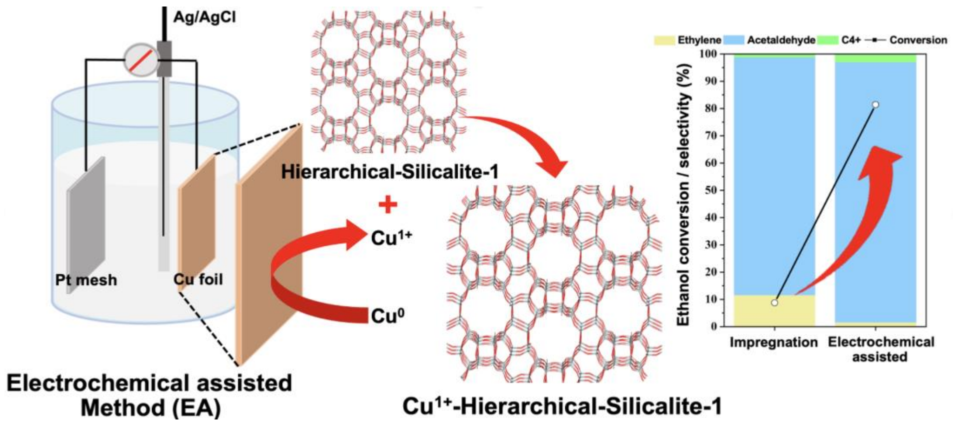
Acetaldehyde is one of the promising intermediate chemicals that is widely used in pharmaceutical and plastic precursor industries. It is primarily produced via ethanol dehydrogenation using a Cu-based catalyst. Although catalysts designed by incorporating metallic Cu supported on various zeolites, especially silicalite-1 and Beta zeolites, have been proposed and reported to be active for ethanol conversion. However, acetaldehyde production still suffers due to low metal dispersion, aggregation, and inactive copper species, eventually reducing catalytic efficiency and leading to rapid deactivation. Therefore, challenges in synthesizing and fine-tuning the effect of Cu active species have been further explored.

This study presents an electrochemical assisted (EA) method to precisely control the formation of Cu^+ active species by applying an electrochemical potential, thereby overcoming these limitations. Monometallic Cu^+ species were loaded on hierarchical silicalite-1 (HieSN-1) via the EA approach and subsequently evaluated for ethanol dehydrogenation. The Cu-HieSN1-EA catalyst achieved approximately 86% ethanol conversion, ~96% acetaldehyde selectivity, and an acetaldehyde yield exceeding 82%. In contrast, the Cu-HieSN1-IMP catalyst exhibited only ~10% conversion, 87% acetaldehyde selectivity.

This enhancement is attributed to the superior dispersion of Cu^+ species facilitated by the EA method. These findings demonstrate that the novel EA approach is highly effective in precisely controlling the formation of active Cu^+ species. This method improves catalytic performance and proposes a perspective for sustainable biomass conversion.

Keywords: electrochemical assisted method; Cu^+ species; Cu-silicalite-1; ethanol dehydrogenation reaction



Catalytic Systems for Contemporary Challenges (S2-P-006)

One-step electrochemical production of ethylene glycol and H_2 using Pd-based electrocatalysts

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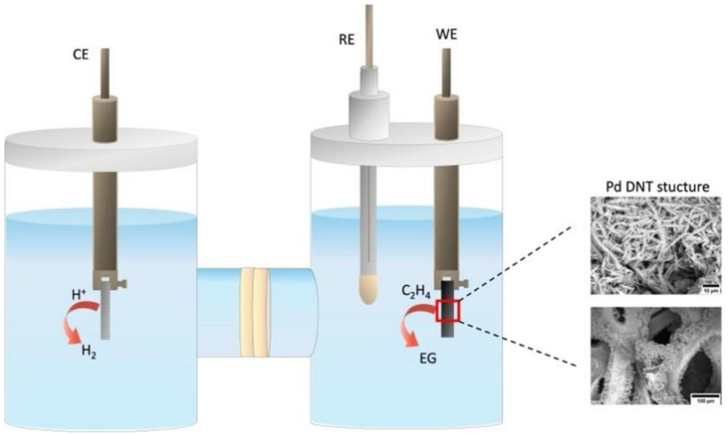
Ethylene glycol (EG) is a vital compound in the petrochemical industry due to its wide range of applications. For example, it is used as a precursor for the synthesis of polyethylene terephthalate (PET), polyester fibers, and automotive antifreeze and coolant. Traditionally, EG is produced from ethylene gas *via* a two-step thermal catalytic process under harsh reaction conditions, accompanied by significant CO_2 emissions. [*J. Am. Chem. Soc.* **2024**, *146*, 5622–5633; *Nat. Catal.* **2023**, *6*, 585–595; *Nat. Catal.* **2020**, *3*, 14–22] To achieve the sustainable scheme, this work introduces the electrochemical synthesis of EG using palladium-based electrocatalysts deposited on Ni foam as a working electrode (WE). To fabricate the WE, the electrodeposition method was carried out yielding the palladium dendritic nanostructured catalyst. Furthermore, an effect of charge density ranging from -4, -6, and -8 C cm^{-2} on electrocatalytic performances was investigated, revealing that the WE obtained at -8 C cm^{-2} exhibited a uniform Pd coverage. In addition, the influence of applied potential on ethylene oxidation was studied. The results show that at a potential of 1.1 V vs. Ag/AgCl, the highest Faradaic efficiency of EG was achieved. Moreover, not only EG was obtained on the anode side, but H_2 gas also was generated on the cathode side. This example opens up perspectives of the simultaneous production of EG and H_2 using a sustainable approach in a one-step process.

Keywords: electrochemical synthesis of EG; ethylene oxidation; green H_2 production



Catalytic Systems for Contemporary Challenges (S2-P-010)

Tuning surface defects and oxygen vacancy concentration in Zr-based MOF derived $ZnZrO_x$ for CO_2 hydrogenation to methanol

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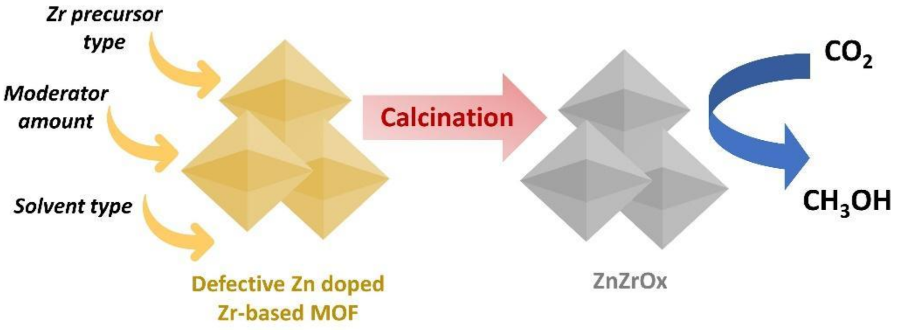
$ZnZrO_x$ with tunable concentration of oxygen vacancies was synthesized via the thermal decomposition of defective Zn-doped Zr-based MOFs for CO_2 hydrogenation to methanol. Zr-based MOFs were prepared using a solvothermal method at 120 °C for 24 hours. The effects of different Zr precursors, moderator amounts, and solvent types on the structural and chemical properties of the resulting $ZnZrO_x$ were investigated. The materials were characterized by XRD, SEM, FTIR, N_2 physisorption, CO_2-TPD, and XPS. XRD and SEM results revealed distinct morphological and structural differences in Zr-based MOFs obtained from $ZrOCl_2·8H_2O$ and $ZrCl_4$. Under similar synthesis conditions, $ZrCl_4$ led to the formation of well-defined octahedral crystals with particle sizes of 100–200 nm, whereas $ZrOCl_2·8H_2O$ yielded rounder particles with much smaller sizes. This observation arises from the rapid nucleation promoted by the direct formation of a hexanuclear secondary building unit of Zr-based MOF through the hydrolysis of $ZrOCl_2·8H_2O$. Consequently, due to the different particle sizes, the derived $ZnZrO_x$ materials exhibited varying contributions of m-ZrO_2 and t-ZrO_2 in their structures. The ability to tune oxygen vacancies and surface defects in $ZnZrO_x$ derived from Zn-doped Zr-based MOFs plays a pivotal role in CO_2 activation and CH_3OH formation.

Keywords: CO_2 conversion; methanol; catalysis; metal-organic framework; metal oxide



Catalytic Systems for Contemporary Challenges (S2-P-011)

Development of zinc indium sulfide photocatalyst for hydrogen production via water-splitting process

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Hydrogen energy is a crucial and clean energy source that does not contribute to environmental pollution. Producing hydrogen through the process of water splitting under visible light is particularly noteworthy because it occurs at low temperatures, uses less energy, and is environmentally friendly. Therefore, this project investigates the effect of the zinc indium sulfide ($ZnIn_2S_4$) catalyst, prepared under varying precursors and conditions, on hydrogen production via water splitting under visible light. Initially, the $ZnIn_2S_4$ catalyst is synthesized from different sulfur (S) precursors, specifically thiourea and thioacetamide, at various synthesis temperatures. The efficiency of hydrogen production through the water-splitting process using a Xe 300 W lamp indicated that the catalyst synthesized with thioacetamide at 140°C ($ZnIn_2S_4$-A140) produced the highest amount of hydrogen. This outcome can be attributed to the better structural integrity of $ZnIn_2S_4$ and a smaller bandgap in the $ZnIn_2S_4$-A140 catalyst, which enhanced the absorption of visible light and the efficiency of electron excitation from the valence band to the conduction band, thereby generating more electron-hole pairs.

Keywords: zinc indium sulfide; photocatalysis water splitting reaction; sulfur precursor; visible light

Catalytic Systems for Contemporary Challenges (S2-P-012)

NH_3 synthesis from H_2O and N_2 using an electrochemical cell with Ru catalysts and alkaline metal hydroxide electrolytes

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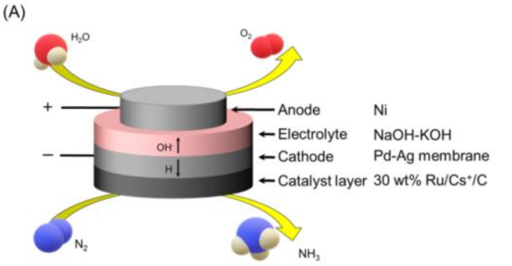
Renewable energy sources such as wind and solar power have the potential to play a vital role in achieving a carbon-neutral society. However, they are inherently unstable due to weather fluctuations, and converting excess energy into chemical energy carriers is essential to prevent waste. Ammonia (NH_3) is one such chemical energy carrier, gaining attention as a carbon-free fuel used in engines, turbines, and fuel cells, as well as a raw material in the production of fertilizers and plastics. This research explores NH_3 synthesis from water (H_2O) and nitrogen (N_2) using electrochemical cells with molten NaOH-KOH electrolytes and $Ru/Cs^+/C$ catalysts at 250 °C and 1.0 MPa. Instead of directly reducing N_2 electrochemically, this process uses catalytically activated N_2, leading to significantly improved NH_3 production rates. The system incorporates a refrigerated NH_3 separator and a recirculation pump, achieving a 90% apparent current efficiency and an NH_3 production rate of 320 nmol s^{-1} cm^{-2} at 250 °C, 1.0 MPa and 100 mA cm^{-2}. The remaining 10% of the apparent current efficiency is used to hydrogen (H_2) evolution. These results highlight the potential of adaptable electrochemical NH_3 synthesis powered by renewable energy.

Keywords: ammonia synthesis; alkaline electrolytes; water electrolysis; Ru catalysts; green fuels



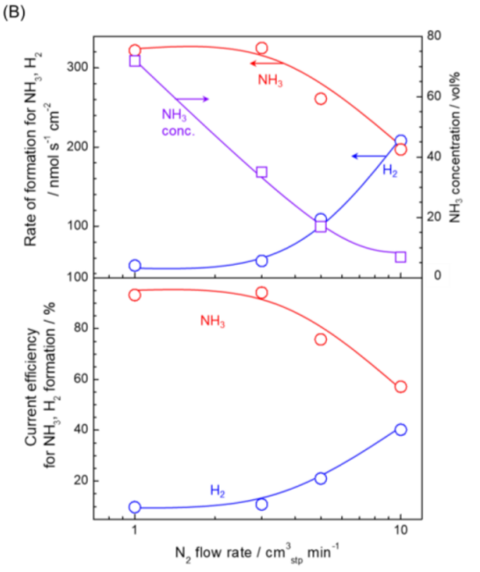


Illustration of present electrochemical cell (A), NH_3 and H_2 formation rates, NH_3 concentration, and apparent current efficiency (B) for NH_3 and H_2 formation from H_2O and N_2 at 250° C and 1.0 MPa with the NH_3 separation at −75° C and unreacted gas recirculation.

Catalytic Systems for Contemporary Challenges (S2-P-015)

Twist-induced enantioselectivity on metal surfaces

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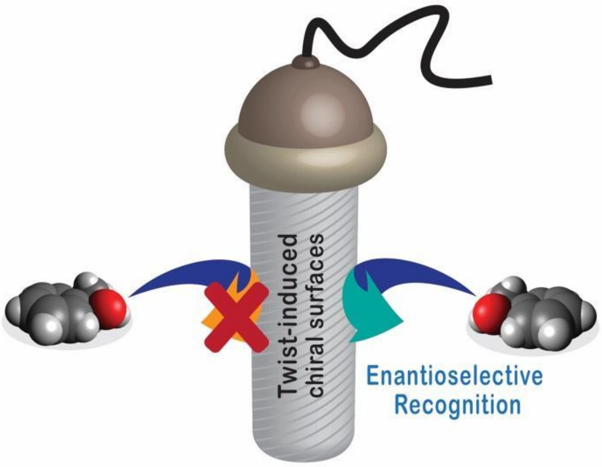
Enantiospecific recognition and synthesis using chiral surfaces can enable enantioselectivity via structure-sensitive surface chemistry. [*Chem. Eur. J.* **2020**, *26*, 2993–3003] Usually, enantiospecific differences in surface reaction kinetics are induced by a chiral environment generated by surface modifications at the molecular or nanometer scale. [*Catal. Lett.* **2015**, *145*, 220–232] However, engineering such well-defined chiral surfaces may encounter some limitations due to complicated preparation steps and the required specific ingredients. In this context, we propose a pioneering approach for creating chiral features on intrinsically achiral metal surfaces via a macroscopic twist. The shear stress generated during the mechanical torsion of a wire in either clockwise (CW) or counterclockwise (CCW) directions facilitates the reorganization of surface atoms, eventually allowing the extrinsic generation of high-Miller-index crystallographic planes which may have chiral features. We were able to demonstrate that such a macroscopic twist allows inducing a certain chiral recognition ability at the molecular level. The respective enantiomers of a chiral molecule are preferentially interacting with wires twisted in opposite directions. In addition to the enantioselective recognition, the twisted metal surfaces ultimately enable also the electrosynthesis of a chiral molecule with a small but significant enantiomeric excess by the reduction of a prochiral precursor. In contrast, no enantiospecificity is observed with untwisted wires.

Keywords: chirality; enantioselective recognition; asymmetric synthesis; chiral metal surfaces



Catalytic Systems for Contemporary Challenges (S2-P-016)

Chiral-induced spin selectivity effect at chiral-encoded Pt-Ir surfaces for enhanced oxygen reduction reaction

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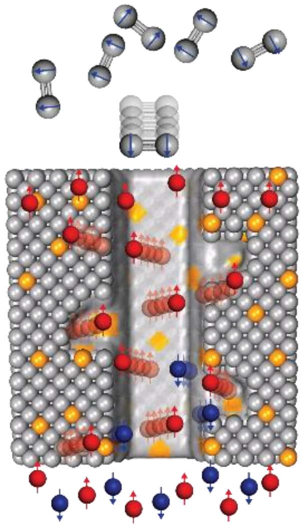
Chiral-induced spin selectivity (CISS) is emerging as a powerful tool for enhancing electrochemical processes, particularly in the oxygen reduction reaction (ORR), which is vital for fuel cells. This work explores the direct application of CISS using intrinsically chiral metal surfaces, instead of the more traditional organic chiral modifiers. [*PNAS* **2022**, *119*, e2202650119] We developed mesoporous Pt-Ir alloys with imprinted chiral information obtained through electrodeposition, in the simultaneous presence of chiral templates. These materials retain their chirality even after complete removal of templates, yielding robust chiral electrodes [*Nat. Commun.* **2021**, *12*, 1314; *Nat. Commun.* **2014**, *5*, 3325; *J. Am. Chem. Soc.* **2019**, *141*, 18870]. Electrochemical studies revealed a significant enhancement in ORR activity when imprinted with one stereoisomer, leading to increased current intensities, compared to achiral analogs or electrodes imprinted with the opposite enantiomer. This demonstrates for the first time the feasibility of leveraging intrinsic metal chirality for CISS-mediated ORR catalysis, offering a novel approach for designing high-performance electrocatalysts for clean energy applications.

Keywords: chiral-induced spin selectivity; oxygen reduction reaction; electrocatalyst; chiral-encoded mesoporous metal



Concept of the CISS effect on Chiral-encoded Pt-Ir surfaces

Hierarchical ZSM-5@NiCoAl layered double hydroxide nanocomposites: Synthesis, characterization, and application in ethane production from CO_2

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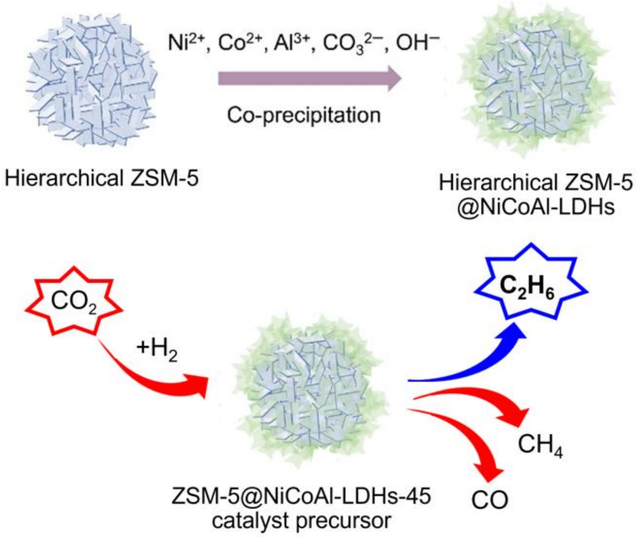
Achieving highly dispersed metal nanoparticles on solid supports remains a major challenge due to metal agglomeration, which reduces catalytic performance. To address this, we report a strategy for synthesizing NiCo species supported on hierarchical ZSM-5 nanosheets using a NiCo-layered double hydroxide (LDH) precursor grown *in situ* on the ZSM-5 surface. The effect of varying the NiCo-LDH to ZSM-5 weight ratio was explored, with 45 wt.% loading (ZSM-5@NiCoAl-LDHs-45) identified as optimal. This composite exhibited a high BET surface area of 386 $m^2 g^{-1}$, with enhanced metal–support interaction and a favorable distribution of micro- and mesopores. The catalyst demonstrated effective CO_2 hydrogenation to ethane at 380 °C and ambient pressure, achieving up to 40% CO_2 conversion at a WHSV of 2.91 h^{-1}. Ethane selectivity reached at ~45% at a higher WHSV of 21.81 h^{-1}. Furthermore, the catalyst maintained stable ethane production over 24 hours of time-on-stream. These results highlight the potential of LDH-derived bimetallic systems on hierarchical zeolites for selective and stable CO_2 conversion.

Keywords: hierarchical ZSM-5; NiCo-LDHs; composite; CO_2 methanation



AI in Drug Discovery Research (S5-P-003)

Preclincial invesitgation of a novel curcumin analogs (dibenzylidene-acetones) as a therapeutic drug for head and neck squamous modulating CXCL10/STAT1/FN1 signaling network

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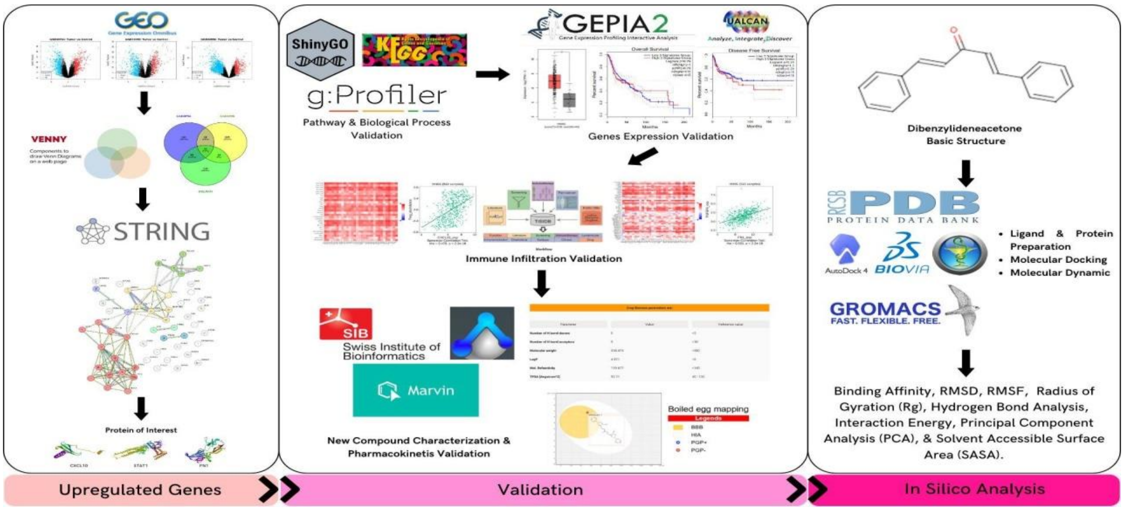
In Indonesia, head and neck squamous cell carcinoma (HNSCC) is an important public health problem, displaying diverse incidence rates and clinical features. The prevalence of HNSCC cases is anticipated to increase around 30% by 2030. A key issue is the recurrent late-stage diagnosis, primarily due to limited cancer awareness, socioeconomic, and reliance on alternative medicine. These factors collectively result in suboptimal treatment outcomes and reduced survival rates. This study examined on efficacy of curcumin analogs in treating HNSCC by supressing CXCL10, STAT1, and FN1. GEO databases were scanned for upregulated genes to evaluate gene expression and immune infiltration. To validate, CXCL10, STAT1, and FN1 were docked with Dibenzylideneacetone (DBA) as curcumin analog. The study found that HNSCC tissues expressed more CXCL10, STAT1, and FN1 than normal tissues. Overexpression of these proteins have correlation with inflammation, especially immune-mediated expression. Molecular docking showed better binding affinities than traditional treatment. The study found elevated gene signatures (CXCL10, STAT1, and FN1), immune infiltration profiles, and prospective HNSCC treatment candidates, demonstrating DBA's inflammatory pathway inhibition. Data collection will continue using molecular dynamics.

Keywords: HNSCC; DBA; curcumin analogs; CXCL10/STAT1/FN1; *in silico* analysis



AI in Drug Discovery Research (S5-P-009)

Computational investigation of the Ru-mediated preparation of benzothiazoles from *N*-arylthioureas: Elucidation of the reaction mechanism and the origin of differing substrate reactivity

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Benzothiazoles are important heterocyclic compounds found in a wide range of pharmaceutically active agents and natural products. Transition-metal-catalyzed methods have been widely used for the synthesis of benzothiazoles via intramolecular C−S bond formation. This prompted the preparation of benzothiazoles from ortho-haloarene precursors catalyzed by ruthenium-based complex with differing yields and selectivities depending on the substrate in question. In this work, we employed a density functional theory-based computational model to investigate the reaction mechanism leading to the desired benzothiazole product, as well as uncover the origin of the differing yields and selectivities observed experimentally. We have identified the rate determining step associated with the reaction mechanism using UB3PW91/6-31+G(d,p) for all atoms except ruthenium (LanL2DZ). The rate determining step was found to be H^-/H^+ transfer reaction in TS1 with the energy barrier of 16.2 kcal/mol. This is consistent with the experimental observed kinetic isotope effects. The theoretical results in the examination of the influence of electron donating and electron withdrawing groups substituent on the different positions of the N-arylthioureas can prove useful to explore the reaction further.

Keywords: benzothiazoles; ruthenium; mechanism; DFT; arylthioureas

AI in Drug Discovery Research (S5-P-010)

Rational design of InhA inhibitors from Thai natural products using molecular docking calculation and *ab initio* fragment molecular orbital approach

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Masayuki Yuguchi,[2] Nagomi Chimura,[2] Auradee Punkvang,[3] Khomson Suttisintong,[4]
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Tuberculosis (TB) is a severe infectious disease in humans caused by *M. tuberculosis*. The enzyme enoyl-acyl carrier protein reductase (InhA) plays a crucial role in the biosynthesis of mycolic acids, which are essential for the survival of *M. tuberculosis*. As a result, InhA is a promising target for antituberculosis drug development. In this study, we investigated the key interactions between InhA and six Thai natural products: 3NP, Brazilin, Methyl gallate, Eugenol, α-Mangostin, and Damnacanthal. These compounds were previously isolated in our research, we demonstrated their potential inhibitory activity against InhA, highlighting them as promising candidates for further exploration as antitubercular agents. To better understand the variations in their inhibitory effects, molecular docking calculations were performed to analyze their binding modes and interactions within the InhA binding pocket. Additionally, *ab initio* fragment molecular orbital calculations were conducted on the complex structures to evaluate binding energies and key interactions between the ligands and InhA. The total interaction energies of ligand ranged from −33.7 to −72.1 kcal/mol. The most potent compound exhibited strong interactions with InhA, specifically with Ala157 and Gln213. Finally, the results provide valuable insights for the rational design of more potent InhA inhibitors with effective anti-tuberculosis activity.

Keywords: *Mycobacterium tuberculosis*; InhA; molecular docking calculations; *ab initio* fragment molecular orbital calculations; specific interactions

AI in Drug Discovery Research (S5-P-011)

Quantitative structure activity relationship and molecular docking calculations of xanthone derivatives as anti-tuberculosis agents

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Tuberculosis (TB), caused by *Mycobacterium tuberculosis*, remains one of the most widespread diseases globally. A major challenge in TB treatment is the mutation of the DNA gyrase enzyme, which contributes to drug resistance. Consequently, there is an urgent need to discover novel and potent DNA gyrase inhibitors to overcome this resistance. Xanthone derivatives have emerged as promising GyrB inhibitors with potential anti-tuberculosis activity. In this study, molecular docking calculations were conducted to explore the binding modes and interactions of these derivatives. The results indicate that hydrogen bonding occurs between the oxygen atom at the R position of the ligand and the hydrogen atoms of Asp79, Thr169, and Gly83. Additionally, xanthone derivatives exhibited π-cation interactions between their benzene ring and Arg82, π–π interactions with Pro85 at the R' position, and π–sigma interactions with Glu56 and Ile84. Van der Waals interactions were also observed with Asn52 at the R'' position of the ligand. The QSAR model obtained is statistically reliable. These combined results contribute to the rational design of new, more potent GyrB inhibitors for tuberculosis treatment.

Keywords: *Mycobacterium tuberculosis*; GyrB; structure-quantitative activity relationship; molecular docking calculations; xanthone derivatives

AI in Drug Discovery Research (S5-P-012)

Harnessing artificial intelligence for drug discovery: Opportunities and impact in South Africa

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The integration of artificial intelligence (AI) into drug discovery has revolutionized the pharmaceutical landscape, offering accelerated timelines, enhanced accuracy, and reduced costs. In the South African context, where the burden of communicable and non-communicable diseases remains high and research infrastructure is developing, AI presents a transformative opportunity. This study explores the current and potential impact of AI-driven drug discovery within South Africa, focusing on machine learning algorithms for target identification, molecular screening, and predictive pharmacology. Through a synthesis of existing applications, including local initiatives leveraging AI to combat tuberculosis and HIV, we examine how AI tools are tailored to regional disease profiles and resource constraints. Challenges such as data scarcity, limited computational infrastructure, and regulatory uncertainties are discussed alongside strategies for capacity building and collaboration. The findings highlight that while AI adoption in South African drug discovery is nascent, strategic investments and policy support could position the country as a regional hub for AI-driven biomedical innovation. These abstract underscores the need for inclusive, equitable AI frameworks that address both global innovation and local healthcare priorities

Keywords: artificial intelligence; drug discovery; South Africa; machine learning

AI in Drug Discovery Research (S5-P-013)

Investigation of the bioactivities of *Caesalpinia pulcherrima* (L.) SW wood extracts and *in silico* analysis of stigmasterol as an InhA inhibitor_

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This research evaluates the chemical constituents, antioxidant activity, and antibacterial activity of crude extracts from the wood of *Caesalpinia pulcherrima* (L.) SW. Additionally, molecular simulations were performed. Crude extracts were obtained using hexane, dichloromethane, ethyl acetate, and methanol. The methanol extract yielded the highest percentage at 0.64%. Antioxidant activity was assessed using the ABTS assay at a concentration of 1000 mg/L of the ethyl acetate extract, resulting in 14.61% ± 1.31 inhibition. Antibacterial activity was evaluated using the agar disc diffusion method at concentrations of 200, 500, and 1000 mg/mL. The ethyl acetate extract at 1000 mg/mL showed an inhibition zone of 8.33 ± 0.58 mm against S. aureus ATCC 25923. Stigmasterol was identified in the ethyl acetate extract, and its inhibition of InhA was assessed, showing 95% inhibition at 64 µM. To further investigate its inhibitory mechanism, molecular docking was conducted to analyze binding modes and interactions within the InhA binding pocket. Stigmasterol exhibited the lowest binding energy at −4.77 kcal/mol. The most active compound formed strong interactions with InhA, including hydrogen bonds with Asp150 and Arg153. These findings provide valuable insights for the rational design of more effective InhA inhibitors with enhanced anti-tuberculosis activity.

Keywords: *Caesalpinia pulcherrima*; stigmasterol; antioxidant activity; antibacterial activity; molecular docking calculations

AI in Drug Discovery Research (S5-P-015)

Investigation of covalent inhibitors of protein kinases using QM/MM calculations

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Non-small cell lung cancer (NSCLC) is the type of lung cancer that causes the most deaths annually. Epidermal growth factor receptor (EGFR) is a receptor tyrosine kinase implicated in the uncontrolled cell growth associated with NSCLC and has prompted the development of multiple EGFR inhibitors to treat the disease. Drug discovery efforts on this target initially focused on traditional reversible ATP-binding site inhibitors, however irreversible covalent binding EGFR inhibitors have become increasingly more popular. Covalent EGFR inhibitors have been developed using a range of different scaffolds and, unsurprisingly, the incorporation of an electrophilic acrylamide group can result in sizeable orientation differences relative to the Cys797 nucleophile and the Asp800 general base. In this work, we report a QM/MM study aiming to better understand aspects of covalent adduct formation, including the role of protein flexibility on chemical reactivity, the impact electrophile location within the ATP binding site, as well as the impact of the acrylamide conformation (s-cis vs s-trans). We focus here on the diaminopyrimidine scaffold, as exemplified by Rocelitinib, where the electrophile is attached to its back pocket binding group. Our goal is to shed greater light on how electrophilic groups can be incorporated onto different inhibitor scaffolds targeting reactive active site residues. We find that irrespective of the EGFR MD conformation chosen investigated, acrylamide in both the s-cis or s-trans can react with a rate-determining barrier of ~20 kcal/mol in line with experimental expectations. Interestingly, the nature of rate determining step for Rocelitinib-like inhibitors was found to be either direct nucleophilic attack, or keto-enol tautomerization, depending on the precise protein and inhibitor conformation.

Keywords: EGFR, QM/MM, kinase, covalent inhibitor, cysteine

AI in Drug Discovery Research (S5-P-016)

Computational study on binding investigation of 4-isochromanone derivatives as acetylcholinesterase (AChE) inhibitors

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Acetylcholinesterase (AChE) is involved in the hydrolysis of acetylcholine in the central nervous system (CNS), contributing to the development of Alzheimer's disease (AD). Recently, the 4-isochromanone derivatives have been indicated as potent AChE inhibitors, demonstrating efficient experimental IC_{50} values in low nanomolar units. To elucidate the excellent inhibition against AChE activity. Therefore, this work has explored the binding modes of these derivatives through computational studies such as molecular docking, molecular dynamics (MD) simulations, and quantum chemical calculations (QCC). The equilibrium structures of AChE and these derivatives from MD simulations exhibit pi-pi and hydrogen-pi interactions with Trp286, occurring exclusively between the aromatic ring and the methoxy group of the 4-isochromanone moiety in the derivatives. Additionally, a pi-pi interaction is observed with Tyr341 through the aromatic part of the 4-isochromanone structure. Trp286 and Tyr341 are identified as the key residues of the derivatives within AChE. Furthermore, ADMET predictions indicated that all compounds enhance acceptable properties to be considered promising drug candidates. Consequently, computational studies have confirmed the 4-isochromanone derivatives as a promising scaffold for future AChE drug development.

Keywords: Alzheimer’s disease; acetylcholinesterase; MD simulations; quantum chemical calculations; ADMET predictions

AI in Drug Discovery Research (S5-P-017)

A computational study on the binding of diterpene lactone derivatives with the main protease (M^{pro}) of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2)

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The main protease (M^{pro}) plays a critical role in viral replication and a promising target for antiviral drug development. This study investigates the binding interactions between SARS-CoV-2 M^{pro} and five diterpene lactones from *Andrographis paniculata*: andrographolide (AP1), 14-deoxy-11,12-didehydroandrographolide (AP2), neoandrographolide (AP3), 14-deoxyandrographolide (AP4), and 14-deoxy-14,15-didehydroandrographolide (AP5). Molecular dynamics (MD) simulations of 200 ns were conducted to evaluate the stability and binding affinity of the complexes. Principal component analysis (PCA) and free energy landscape (FEL) analysis were investigated to confirm the structural stability and equilibrium of the systems. Binding free energies were determined using molecular mechanics Poisson-Boltzmann surface area (MM-PBSA) and quantum mechanical (QM/MM) approaches. From the results, AP3 exhibited the strongest binding affinity, with the lowest binding energy (–31.5 kcal/mol) and the most favorable interaction energy (–44.1 kcal/mol). The residual interaction energies indicated the strong interactions through the hydrogen bonds, π–alkyl, and π–π interactions with the subsites in the M^{pro} binding pocket. These results suggest that AP3 is a promising candidate for further development as a potential SARS-CoV-2 M^{pro} inhibitor, providing valuable insights into the design of therapeutic agents against COVID-19.

Keywords: SARS-CoV-2 M^{pro}; *Andrographis paniculata*; diterpene lactones; MD simulations; QM/MM

AI in Drug Discovery Research (S5-P-018)

Virtual screening and computational analysis of *Styrax tonkinensis* compounds targeting acetylcholinesterase

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Alzheimer's disease, a primary contributor to dementia, mainly affects the elderly but can also occur in younger individuals due to stress and lack of rest, causing progressive cognitive impairment. Promoting the activity of acetylcholinesterase (AChE), which regulates acetylcholine (ACh) breakdown, a neurotransmitter. It is linked to cognitive decline in Alzheimer's. This study focuses on AChE, the key enzyme responsible for the breakdown of acetylcholine. It investigates compounds derived from *Styrax tonkinensis*, a plant known for its beneficial effects on the nervous system. Active compounds were found, and their interactions with AChE were studied using molecular dynamics (MD) simulations and quantum chemical calculations. Tonkinensisin-A demonstrated the highest docking score. MD simulations indicated that this compound was stable and interacted with key residues in the binding site through the pi-alkyl and pi-pi interactions with TRP286 and TYR341, respectively, similar to donepezil. MM-PBSA, MM-GBSA, and QM/MM calculations revealed that Tonkinensisin-A had lower binding and interaction energies than donepezil. The stability of the complex was confirmed by the principal component analysis (PCA) and free energy landscape (FEL) analysis. As a result, Tonkinensisin-A could serve as a promising candidate for further study into the mechanisms of AChE inhibition.

Keywords: Alzheimer's disease; acetylcholinesterase; molecular dynamics simulations

AI in Drug Discovery Research (S5-P-019)

Structure-based virtual screening of traditional Thai remedy Prabchompoothaweep for novel acetylcholinesterase inhibitors

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Alzheimer's disease (AD) is a major neurodegenerative disorder, and current acetylcholinesterase (AChE) inhibitors have limited efficacy and notable side effects. As a result, natural products are being explored as safer, more selective alternatives. The Prabchompoothaweep remedy, a traditional Thai formulation of 23 herbs, is recognized for its anti-inflammatory and antioxidant properties. This study aimed to identify potential AChE inhibitors from this remedy. Phytochemicals from the 23 herbs were gathered from literature, and five compounds were selected for in silico screening. Molecular dynamics (MD) simulations of 100 nanoseconds were performed on AChE complexes with the selected compounds and compared to the FDA-approved drug donepezil. The results showed that both Donepezil and the selected compounds formed stable bindings within the AChE active site. Principal component analysis (PCA) and free energy landscape (FEL) analysis confirmed the stability of these interactions. Quantum chemical calculations (QCCs) highlighted crucial π–π interactions with Trp86, Trp286, and Tyr341. Phyllanemblinin F exhibited enhanced stability, forming an additional hydrogen bond. Bioavailability predictions suggested favorable pharmacokinetic properties. These findings suggest that phyllanemblinin F could be a promising lead for the development of AChE inhibitors for AD therapy.

Keywords: acetylcholinesterase; natural compounds; molecular dynamics (MD) simulations; quantum chemical computations

AI in Drug Discovery Research (S5-P-020)

Machine learning assisted *in-silico* and *in-vitro* investigation of the synergistic and antagonistic effects of essential oils against *Staphylococcus aureus*

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Antibiotic-resistant *Staphylococcus aureus* presents a significant health challenge, necessitating alternative antimicrobial solutions. This study investigates the synergistic and antagonistic effects of ten selected essential oils against *S. aureus* using an integrated approach of machine learning, *in-silico*, and *in-vitro* methods. Graph embedding was used to model interactions among 147 compounds in the essential oils, followed by multinomial logistic regression to classify interactions as synergistic, antagonistic, or neutral and model predicted forty-five synergistic and antagonistic interaction pairs. *In-vitro* antibacterial studies were conducted using microdilution method. Molecular docking was used to explore binding interactions with key *S. aureus* proteins: Sortase-A, DNA Gyrase, and Dihydrofolate Reductase, while molecular dynamics (MD) simulations were conducted exclusively for DNA Gyrase. MM/PBSA and MM/GBSA free energy calculations were utilized to rank ligand binding affinities and predict interaction stability. The essential oils of bark and leaves of *Cinnamomum zeylanicum* exhibited the highest antibacterial activity with minimum inhibitory concentrations (MIC) of 0.50 mg/mL and 0.25 mg/mL respectively. Diallyl trisulfide emerged as the most promising compound with strong binding affinity against DNA Gyrase. Further model development and in-vitro validation are recommended to fully explore the therapeutic potential of essential oils against *S. aureus.*

Keywords: essential oils; synergism; *Staphylococcus aureus*; machine learning; molecular docking; molecular dynamics

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-P-002)

Bioactive extraction from bamboo, roselle, and monk fruit for a fiber-rich wellness drink with sustainable packaging

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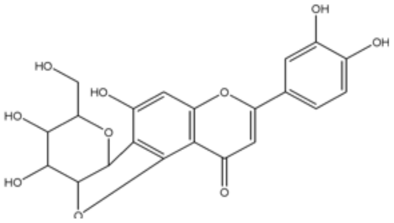
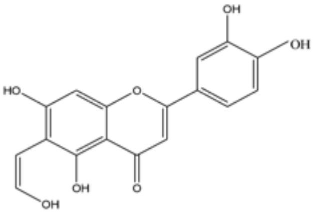
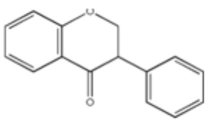
This study investigates the extraction, characterization, and application of bioactive compounds from various species of bamboo (Bambusoideae), with an emphasis on optimizing the retention and controlled release of flavonoid-rich extracts for multifunctional use. Eight bamboo species were evaluated for agronomic performance and phytochemical composition, with *Dendrocalamus sericeus* Munro (Sang-Mon bamboo) exhibiting the highest total flavonoid content, reaching a peak during the post-monsoon period (October–November). Flavonoid structures were elucidated using UV-Vis spectroscopy and HPLC analysis. Antibacterial assays demonstrated significant inhibition zones against *Staphylococcus aureus* and *Escherichia coli,* while cytotoxicity assessments confirmed the safety of the extracts at concentrations below 100 ppm in fibroblast cell lines. In addition, silver nanoparticles synthesized via green methods using Sang-Mon bamboo flavonoids exhibited enhanced antioxidant activity, as measured by DPPH and ABTS radical scavenging assays. Encapsulation using lysosome-mimetic vesicles enabled sustained release, indicating strong potential for cosmetic and biomedical applications. These findings contributed to the formulation of a fiber-enriched instant wellness beverage, combining bamboo leaf extract, *Hibiscus sabdariffa* (roselle), *Siraitia grosvenorii* (monk fruit), and citrus-derived soluble fiber. The beverage is designed to support digestive health, metabolic balance, muscle recovery, and hydration. Advanced eco-friendly extraction and encapsulation technologies were employed to preserve bioactivity and improve nutrient bioavailability. The final product offers a sustainable, plant-based alternative to synthetic sports drinks, addressing consumer demand across ASEAN and global markets while enhancing socio-economic opportunities for local agricultural communities through value-added bamboo-based innovations.

Keywords: bamboo leaf extract; flavonoids; antioxidant; antibacterial







Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-P-003)

Preparation of bioactive ionic liquids for extraction of polyhydroxylated fatty alcohols from avocado (*Persea americana*)

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Ionic liquids have emerged as a promising and sustainable alternative to conventional solvents in response to increasing concerns over the environmental and health hazards associated with traditional methods used for the extraction of bioactive natural products. Ionic liquids have interesting properties including tunability and recyclability. In this study, cholinium-based ionic liquids were synthesized and evaluated as an extraction solvent system, in combination with co-solvents, e.g., water, ethanol, and hexane, for the extraction of virucidal polyhydroxylated fatty alcohols from the seeds and pulp of *Persea americana* (avocado). Although the synthesized cholinium-based ionic liquids could extract polyhydroxylated fatty alcohols from the avocado matrix under the tested conditions, separation of the ionic liquids from co-solvents was difficult, and thus hampering the recycling of ionic liquids. Therefore, these ionic liquids may not be suitable for the extraction of bioactive natural products. However, we found that some ionic liquids exhibited antibacterial activity against the selected bacterial strains, suggesting potential utility in antimicrobial applications.

Keywords: ionic liquid; cholinium-based ionic liquids; polyhydroxylated fatty alcohols; avocado; *Persea americana*

Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-P-004)

Determination of chemical constituents and biological activity from crude extract of wood of *Caesalpinia pulcherrima* (L.) Sw.

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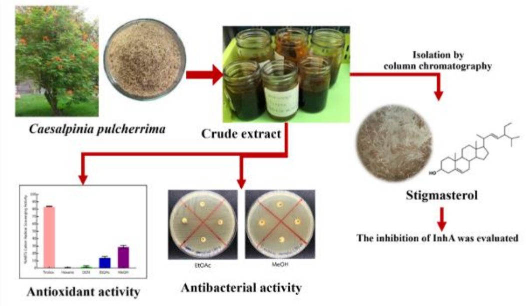
In recent years, plant-based treatments for various diseases have garnered significant attention due to their therapeutic potential. Bioactive compounds extracted from plants have demonstrated promising applications in the medical field. One such plant of interest is *Caesalpinia pulcherrima* (L.) SW. This study aimed to evaluate the chemical constituents, antioxidant activity, and antibacterial properties of crude extracts obtained from the wood of *Caesalpinia pulcherrima*. Extractions were carried out using hexane, dichloromethane, ethyl acetate, and methanol, with the methanol extract yielding the highest efficiency at 0.64%. Antioxidant activity was measured using the ABTS assay at a concentration of 1000 mg/L, resulting in an inhibition rate of 29.32 ± 1.49%. Antibacterial activity was as evaluated. At 1000 mg/mL, both ethyl acetate and methanol extracts exhibited inhibition zones against *Staphylococcus aureus* ATCC 25923, with inhibition zones of 8.33 ± 0.58 mm and 7.50 ± 0.71 mm, respectively. Furthermore, stigmasterol was identified in the dichloromethane extract. Its inhibitory activity against the InhA enzyme was evaluated, showing 95% inhibition at a concentration of 64 μM. These findings indicate that the methanol extract of *Caesalpinia pulcherrima* possesses promising biological activity. Further purification and characterization of its active constituents may enhance its therapeutic potential and support the development of high-value natural products from Thailand.

Keywords: *Caesalpinia pulcherrima*; antioxidant activity; antibacterial activity; chemical constituents; natural products



Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-P-005)

Shellfish “Royal Purple” pigment discovered via HPLC on a 2,500-year old marble jar of the Persian King Darius the Great

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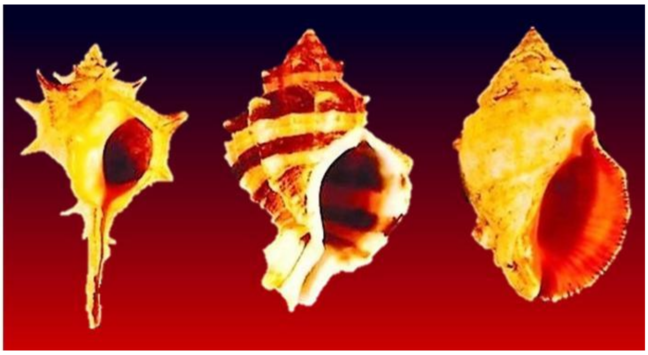
Royal Purple (or Shellfish Purple) is a designation used to describe regal textiles dyed with the purple pigment extracted from a certain gland of some Muricidae sea snails inhabiting the Mediterranean. These purple and violet garments conferred upon the wearer an aura of power and sacredness and, thus, only sovereigns, military generals, eminent officials, and high priests wore such textiles. This molluskan pigment is the most mystifyingly complex of all the natural colorants used in antiquity. In the current research, high-performance liquid chromatography (HPLC) coupled with photodiode array (PDA) detection was used for the microchemical analysis of residual decorative purple paint pigments on the surface of a 2,500-year old stone jar. This pear-shaped marble vessel contains carved quadrilingual inscriptions praising the Persian King Darius I. The major colorants identified in the purple pigment are 6,6'-dibromoindigo, 6-monobromoindigo, and 6,6'-dibromoindirubin, with traces of indigo and 6-bromoisatin. This analysis establishes that a marine mollusk was the source of the purple pigment, which is also known as Tyrian Purple of the ancients – a rare find. A comparison with the relative dye compositions of various Muricidae species suggests that the biological provenance of this ancient pigment was probably an indigo-deficient *Hexaplex trunculus* sea snail.

Keywords: dibromoindigo; monobromoindigo; indigo; *Hexaplex trunculus*; Muricidae



Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia (S6-P-016)

Green synthesis of silver nanoparticles using *Morus alba* Linn. leaf extract and their antibacterial activity

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In this study, environmentally friendly silver nanoparticles (AgNPs) were synthesized using herbal extracts derived from the leaves of *Morus alba* Linn. The objective was to investigate the synthesis process and evaluate the antibacterial efficacy of the AgNPs against *Staphylococcus aureus* (*S. aureus*) and *Escherichia coli* (*E. coli*). The synthesis was carried out by mixing a 0.5% w/v concentration of *Morus alba* Linn. leaf extract with 2 mM silver nitrate at 70 °C for 15 minutes. The successful formation of AgNPs was indicated by a color change from light yellow to dark brown and further confirmed by UV–visible spectrophotometry, which showed a maximum absorption peak at 433 nm. The antibacterial activity of the synthesized AgNPs was assessed using the agar disc diffusion method, resulting in an inhibition zone of 8.33 ± 0.58 mm for *E. coli*, while no inhibition was observed for *S. aureus*. These findings demonstrate the potential of agricultural waste, such as *Morus alba* Linn. leaf, for the green synthesis of AgNPs. Moreover, the synthesized nanoparticles exhibit promising antibacterial properties, paving the way for their application in sustainable antimicrobial development and the value-added utilization of agricultural waste.

Keywords: silver nanoparticles; green synthesis; antibacterial activity; *Morus alba* Linn.

Antioxidant and antibacterial evaluation of chitosan-stabilized silver nanoparticles synthesized through a green approach for potential biomedical applications

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Green synthesis offers an eco-friendly approach to producing silver nanoparticles using natural substances without harmful chemicals. In this study, chitosan, a biodegradable polymer derived from chitin served as both the reducing and stabilizing agent, preventing aggregation of chitosan- silver nanoparticles (CS-AgNPs). CS-AgNPs were characterized using UV-Visible spectroscopy, showing surface plasma resonance at 434 nm. Transmission Electron Microscopy (TEM) analysis revealed predominantly spherical, well-dispersed particles with an average size of 15.68 nm. Fourier Transform Infrared Spectroscopy analysis (FTIR) confirmed the presence of hydroxyl (3200–3600 cm^{-1}), amine (3300–3500 cm^{-1}), and carbonyl (1650–1750 cm^{-1}) groups. Antioxidant activity of CS-AgNPs was assessed using the DPPH (2,2-diphenyl-1-picrylhydrazyl) assay, with methanolic solutions of varying concentrations. Maximum scavenging of 16.45% was observed at 500 µg/mL, with an IC_{50} of 1579.41 µg/mL (SD = 6.06), a significant correlation between concentration and inhibition ($p < 0.05$) confirmed a concentration dependent response. Compared to ascorbic acid, which showed over 75% inhibition across all concentrations, CS-AgNPs demonstrated moderate antioxidant potential. The antibacterial activity of CS-AgNPs was evaluated using the disc diffusion method against Staphylococcus aureus and Escherichia coli. Zones of inhibition indicated effective bacterial suppression. These findings highlight the potential of green-synthesized silver nanoparticles for medical and cosmetic applications due to their combined antioxidant and antibacterial properties.

Keywords: chitosan; silver nanoparticles; antioxidant; antibacterial

Catalytic ethanol dehydration to ethylene over zeolite A synthesized from sugarcane bagasse ash

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The catalytic dehydration of ethanol to ethylene is a crucial process in the petrochemical industry, as ethylene serves as a key building block for various derivatives such as polyethylene, ethylene glycol, ethylbenzene, and styrene. In this study, sugarcane bagasse ash waste from the Mitr Phol Sugar Factory in Amnat Charoen Province, Thailand, was utilized as a feedstock to synthesize zeolite A via the hydrothermal method. The study aims to evaluate the catalytic performance of zeolite A derived from sugarcane bagasse ash as a heterogeneous catalyst for the dehydration of ethanol to ethylene. The catalysts were characterized using XRD, SEM-EDX, FTIR, and N_2 adsorption-desorption analysis. For the catalytic test, zeolite A was used in gas-phase ethanol dehydration at temperatures ranging from 200 to 400 °C. The results revealed that ethylene conversion, selectivity, and yield increased as the reaction temperature rose from 200 to 400 °C. Zeolite A from sugarcane bagasse ash exhibited high acidity, as measured by NH_3-TPD, resulting in 61.9% conversion, 87.7% selectivity, and 54.3% yield toward ethylene at 400 °C. The heterogeneous catalyst, zeolite A from sugarcane bagasse ash, demonstrates significant potential for the efficient dehydration of ethanol to ethylene.

Keywords: sugarcane bagasse ash; zeolite A; dehydration; ethanol; ethylene

Green synthesis of silver nanoparticles using crude extract from peels of *Musa ABB cv. Kluai 'Namwa'* for antibacterial activity

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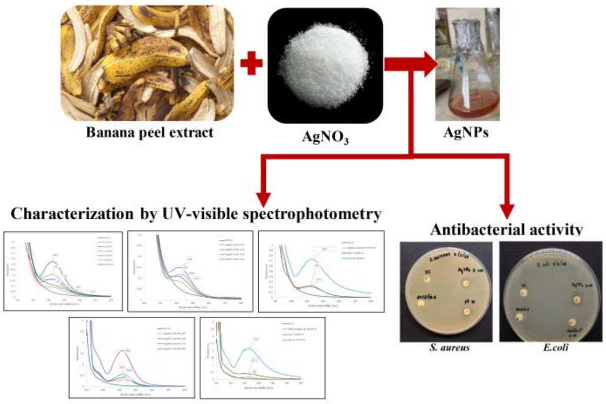
In this study, environmentally friendly silver nanoparticles (AgNPs) were synthesized using herbal extracts derived from the peels of *Musa ABB* cv. *Kluai 'Namwa'*. The synthesis process, along with key parameters—including silver nitrate ($AgNO_3$) concentration, temperature, and solution pH—was systematically investigated. Optimal conditions for AgNP synthesis were identified as 5 and 10 mM $AgNO_3$ at 80°C, with pH values of 5.5 (the original pH before adjustment) and 10. The successful formation of AgNPs was indicated by a visible color change from light yellow to dark brown and confirmed through UV–Visible spectrophotometry, which showed a maximum absorption peak between 412 and 442 nm. The antibacterial activity of the synthesized AgNPs against Staphylococcus aureus and *Escherichia coli* was assessed using the agar disc diffusion method, revealing inhibition zones of 10.00 ± 0.00 mm for both bacterial strains. These findings highlight the potential of agricultural waste, such as banana peels, for the green synthesis of AgNPs. Furthermore, the synthesized nanoparticles demonstrated promising antibacterial properties, supporting their potential application in sustainable antimicrobial development and the value-added utilization of agricultural by-products.

Keywords: silver nanoparticles; banana peels; green synthesis; antibacterial activity;
Musa ABB cv. Kluai 'Namwa'



Activated carbon from sugar cane as an adsorbent of Ca^{2+} ions in water

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One of the chemical parameters for water quality is the calcium content. The presence of Ca^{2+} ions in high levels of water can cause health problems including urolithiasis and cardiovascular disease. Therefore, the reduce of Ca^{2+} ions must be carried out, one of which is by adsorption. This research was conducted to determine the ability of activated carbon from bagasse to adsorption Ca^{2+} ions in water. Bagasse is converted into activated carbon by dehydration, carbonization, and activation processes. Activated carbon was pyrolyzed at 500°C for 30 minutes and activated using a 5% KOH solution with the help of ultrasonic waves for 45 minutes. The results of the adsorption analysis showed that activated carbon bagasse can adsorb Ca^{2+} ions in water with the highest adsorption capacity of 1.19 mg/g and adsorption efficiency of 59.6% at optimum conditions of pH 6, optimum contact time of 30 minutes, and ion concentration Optimum Ca^{2+} 50 mM. The equilibrium data has the best fit with the Langmuir model with $R^2 = 0.9997$.

Keywords: Calcium ion; activated carbon; sugar cane; adsorption

Green process of indigo production using cellulase and comparative environmental sustainability assessment

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Natural indigo is one of the oldest known dyes for its classical blue hue; extracted from the indigo plant (*Indigofera tinctoria*) via conventional fermentation process, that suffers with low yield, poor quality, and long processing time. Current research explored a sustainable process using *Trichoderma* cellulase on Indigofera tinctoria leaves, that experimentally demonstrated double yield of indigo compared with conventional fermentation on dry basis. Dried *I. tinctoria* leaves treated with cellulase showed higher indican content (i.e. indigo precursor) compared to fresh leaves as it might not be fully released in conventional fermentation. This yield enhancement attributes to simultaneous cellulase action for cell wall breaking to release indican and hydrolyzing indican to indigo. At the same time the purity of obtained crude indigo was also significantly improved.

Comparative cradle-to-grave life cycle assessment (LCA) of natural-indigo production from conventional fermentation and enzymatic hydrolysis processes were performed for production pathway sustainability benchmarking. Environmental aspects for 6 categories were exemplified using four different methodologies. The lower product carbon footprint is the preference of both manufacturers and customers today, and results sought out that enzymatic process has ~50% better footprint for all the assessed indicators. Therefore, the enzymatic process has the potential for developing a sustainable and eco-friendly natural indigo production and eventually supporting green economy.

Keywords: cellulase; enzymatic process; cradle to gate; carbon footprint; LCA

Unlocking the Power of Nature: Cutting-Edge Applications of Natural Products, Biological Chemistry, and Chemical Biology (SE-P-009)

Concise total synthesis of *rac*-betuphenone F and their derivatives

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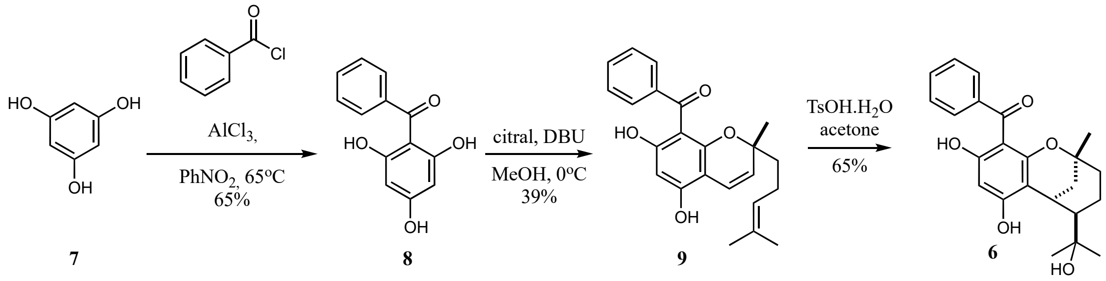
Pancreatic cancer is the most intractable solid cancer with a 5-year survival rate of 10% or less, because early detection is difficult, and it shows resistance to almost all chemotherapeutic agents currently in clinical use. Therefore, there is an urgent need to develop therapeutic agents for pancreatic cancer based on new mechanisms of action not found in existing anticancer agents. Complex natural products with phloroglucinol substructures have long been attractive synthetic targets for synthetic organic chemists. Betuphenone F is a natural product isolated from *Betula alnoides* Ham. ex D. Don (Betulaceae) and structurally determined by S. Awale *et al.* in 2021. Betuphenone F has the potential to be a new-generation anti-cancer agents based on anti-austerity, as it showed preferential cytotoxicity against PANC-1 human pancreatic cancer cells under nutrient-deprived condition. We achieved the first total synthesis of *rac*-bethuphenone F (**6**) from phloroglucinol (**7**) in only three steps. From Friedel-Crafts acylation of phloroglucinol (**7**) follow by treatment with citral using DBU as the base to give the desired cyclization precursor (**9**), then 2-oxabicyclo[3.3.1]nonane skeleton in (**6**) could be easily constructed by adding *p*-TsOH in acetone at low temperature.

Keywords: pancreatic cancer, anti-aussterity strategy, natural product; pholoroglucinol; terpenoid



Science Projects for Students Showcase (SS-P-001)

Cleaning silver jewelry (silver ring) from everyday items using the principles of electrochemistry

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The objectives are to study methods for cleaning black tarnish on silver ring that minimizes silver weight loss, using electrochemical principles and utilize common household items for effective silver jewelry cleaning. The methods: Part 1, prepare silver ring that has black tarnish of Ag_2S . Part 2, find something that can remove the black tarnish on the silver ring. Part 3, the ability to remove black tarnish when using aluminium metal in different sources. Part 4, compare the ability to remove black tarnish of aluminium foil used to wrap food and blister aluminium foil. The results: Part 1, prepare silver ring that has black tarnish of Ag_2S. Put silver rings and boiled eggs in a sealed box. The same black tarnish occurred. Part 2-4, silver ring was in a solution of water: $NaHCO_3$: NaCl: aluminium foil used to wrap food (small pieces) or blister aluminium foil, Ratio 6 mL: 3 coffee spoons: 1 coffee spoon: 1 gram, use hot water it will cause the black tarnish to come off well and cause a chemical reaction to occur quickly. The weight of the silver ring is the same and has a reflectivity similar to the original silver ring. A reflectance value similar to the original silver ring (use RGB Detector application to measure)

Keywords: electrochemistry; silver jewelry cleaning

Science Projects for Students Showcase (SS-P-002)

Living carbonomics: Tracking footprint and storage dynamics above and below ground

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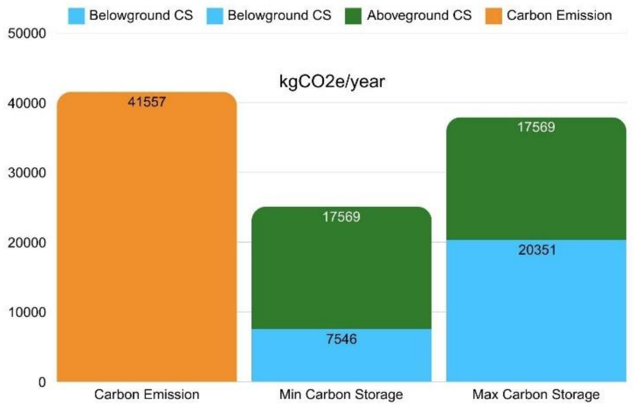
Human-caused disturbances to Earth's carbon equilibrium drive rising global temperatures and increasing climate extremes. This study holistically evaluates carbon dynamics by integrating aboveground and belowground carbon storage, net primary production (NPP), and personal carbon footprint. Aboveground carbon storage was assessed using the Non-Standard Site Carbon Cycle Protocol by measuring 1) tree circumference at breast height (CBH), 2) shrub or sapling height for allometric equations, and 3) herbaceous biomass mass. Belowground carbon storage was estimated using soil bulk density, organic carbon content, soil characterization, and moisture profiles. NPP was evaluated through periodic vegetation growth assessments to incorporate sequestration rates over time. Personal carbon footprint was quantified using the international standard ISO 14064-1:2006 for greenhouse gas reporting. The overall carbon storage, including projected belowground storage, ranged from 25,115 to 37,920 kg, while NPP increased by 202 g C/m^2, reflecting vegetation biomass growth. However, personal carbon footprint rose to 41,557 kg CO2e, surpassing total carbon storage. These findings highlight the imbalance between carbon emissions and sequestration, emphasizing the need for integrated ecological and individual strategies to mitigate climate change through sustainable land use, carbon-conscious practices, and enhanced carbon capture efforts.

Keywords: non-standard site carbon cycle protocol; pedosphere protocol; net primary production; aboveground carbon storage; belowground carbon storage



Science Projects for Students Showcase (SS-P-003)

Study of cardiac troponin I detection using electrochemical sensors based on screen-printed graphene electrodes for assessing the risk of myocardial infarction

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Myocardial infarction is a leading cause of mortality among the working-age population. Diagnosis can be made through an electrocardiogram (ECG); however, additional biomarkers are crucial in cases where the ECG shows no significant changes. One such marker is cardiac troponin I (cTnI), which is highly specific for myocardial infarction. Therefore, this study aims to develop an electrochemical sensor with screen-printed graphene electrodes (SPGEs) for detecting cTnI to assess the risk of myocardial infarction. After electrode fabrication, the SPGE was further anodized in 0.5 M NaOH at a constant potential of +1.3 V for 40 seconds to increase the number of carboxylic groups on its surface. Electrochemical signal responses, such as cyclic voltammetry (CV) and differential pulse voltammetry (DPV), were used to examine surface modifications and determine cTnI levels. Preliminary results revealed that after the anodization step, the current increased compared to the bare electrode, as demonstrated by cyclic voltammograms, while DPV signals decreased as cTnI concentration increased in the range of 0.01 to 1 ng mL^{-1}, with a limit of detection (LOD) of 4.4 pg mL^{-1}. However, further studies will examine variable parameters such as solution pH and incubation time, as well as analytical performance, including linearity and reproducibility.

Keywords: myocardial infarction; cardiac troponin I (cTnI); electrochemical sensors; screen-printed graphene electrode (SPGE)

Science Projects for Students Showcase (SS-P-004)

Spice-relief jelly: "Antioxidant-rich *Carissa* drink with milk casein protein"

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Individuals in Thailand often indulge in spicy delicacies like Somtam, Tom Yum, or Pad Prik Kaeng, which can sometimes be overwhelmingly pungent, leading to discomfort in the mouth, tongue, and stomach due to the fiery nature of capsaicin found in chili peppers. This compound interacts with the protein Casein, effectively numbing the nerve endings responsible for the spicy sensation. Apart from the milk protein's soothing properties, the inclusion of *Carissa carandas*, a fruit renowned for its sweet and tangy flavor, further aids in alleviating the fiery sensation. This fruit boasts numerous benefits, including antioxidants that combat aging, protect against cancer, and provide essential vitamin C for overall well-being.

Inspired by these natural extracts, we conceived a novel product in jelly form aimed at mitigating spicy symptoms. The process involves extracting casein protein from milk and combining it with vinegar to create a powdered form, which is then blended with processed *Carissa carandas*. A gelling agent is incorporated to give the jelly its final shape, followed by assessments using the Dumas combustion to test for casein content, the DPPH method to measure antioxidant activity, user satisfaction evaluations, and efficacy testing of the spicy-reducing effect of the user test by tasters.

Keywords: *Carissa carandas*; casein; capsaicin; jelly; spicy symptoms

Science Projects for Students Showcase (SS-P-005)

Development of paper sensor using dye compound to detect dopamine in sweat for point-of-care diagnosis of parkinson's disease using fluorescent

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Dopamine is an essential biomarker for diagnosing neurological disorders, including Parkinson's disease. Current detection methods are limited by high costs, complexity, and time-intensive sample preparation. This study introduces a novel, cost-effective, and sensitive sensor for dopamine detection using pyrene boronic acid (PBA). The sensor exploits the strong binding affinity between boronic acid and dopamine's diol groups, enabling accurate detection under optimized conditions. Fluorescence spectroscopy confirmed excellent sensitivity and selectivity, achieving a detection limit of 1×10^{-2} M. Experiments revealed that PBA at 1×10^{-3} M could reliably detect dopamine concentrations as low as 1×10^{-2} M. These findings highlight the potential of the PBA-based sensor for real-time dopamine monitoring, paving the way for advancements in biosensing technology and improving accessibility to biomarker detection tools for neurological diagnostics.

Keywords: dopamine; catecholamines; sweat; fluorescent; boronic acid

Science Projects for Students Showcase (SS-P-006)

Preparation of chitosan functionalized rice husk silica employed as drug delivery for folic acid

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In this study, preparing chitosan-functionalized rice husk silica was employed as drug delivery for folic acid. The silica particles were achieved from silica precursor obtained from rice husk. Folic acid was attached to the surface of silica particles through direct bonding and bonding through chitosan. Then, X-ray diffraction, N_2 adsorption-desorption analysis, Fourier transform infrared spectroscopy and scanning electron microscopy were used to study the surface and structure of these composite materials. This was done to confirm that silica particles had a chitosan coating and folic acid conjugation. The chitosan-functionalized rice husk silica exhibited a higher drug loading percentage than the pure rice husk silica. In addition, the effects of the type of silica, pH, time, and temperature on the release of folic acid were also investigated.

Keywords: chitosan; rice husk silica; drug delivery; folic acid

Science Projects for Students Showcase (SS-P-007)

Synthesis of novel activated carbon from longan peel for the removal of caffeine from synthetic hospital wastewater

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This study examined the effect of activation temperature on the physicochemical characteristic of activated carbon derived from longan peel (LPAC). The longan peel was activated with NaOH in different temperatures at 600 and 700 °C. These LPAC materials were then characterized for their surface and structural characteristics using X-ray diffraction, N_2 adsorption-desorption analysis, Fourier transform infrared spectroscopy and Scanning Electron Microscope. The LSAC materials exhibited an amorphous carbon structure, a specific surface area of 1,400.8-2,156.1 m^2/g, an average pore volume of 0.72-1.10 cm^3/g, and an average pore diameter of 9.4-10.2 nm. Moreover, they revealed various types of pore structures. These LPAC materials were used as an adsorbent to remove the caffeine (CAF) from wastewater because CAF in water resources has been reported, indicating the need for alternative treatments. In this study, the LPAC adsorbents evaluated their performance in wastewater with various ions such as synthetic hospital wastewater compared to tap water. In addition, the LPAC with high porosity exhibited the adsorption capacity of CAF more than 120 mg/g.

Keywords: activated carbon; longan peel; caffeine; synthetic hospital wastewater

Production of rayon fibers from used cotton wool and tissue, compared with cellulose fibers from cotton using a small-scale chemical technique

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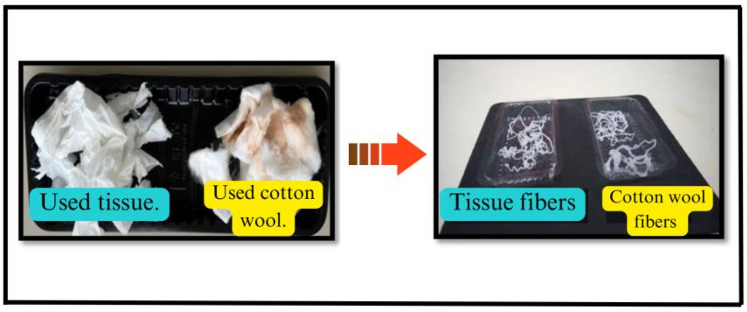
The objectives of this study are 1) To produce rayon fibers from used tissue and cotton wool, as well as fibers from cotton, and fibers with cotton mixed in tissue and cotton wool. 2) To test the properties of these fibers by: preparation of fibers from different materials and testing their properties. Results: 1) Preparation of Fibers**:** Rayon fibers were successfully produced from the selected materials. 2) Testing the Properties of the Fibers: Burning Property: Tissue, cotton wool, and cotton fibers ignited easily with an orange flame and melting, characteristic of rayon. Dye Absorption**:** Pure cotton absorbed the most dye, followed by cotton-wool blended fibers, cotton wool fibers, cotton-tissue blended fibers, and tissue fibers. All fibers maintained color when soaked in water. Water Absorption**:** Pure cotton had the highest water absorption, followed by cotton-cotton wool blended fibers, cotton wool fibers, cotton-tissue blended fibers, and tissue fibers, which absorbed the least. Water Drainage**:** Tissue fibers drained the most water, followed by cotton-tissue blended fibers, cotton wool fibers, cotton-cotton wool blended fibers, and pure cotton fibers.The results demonstrate that fibers from different materials have distinct properties, which can be applied in textiles or related industries. The knowledge gained can be scaled up for larger production of rayon fibers, potentially replacing those made from pure cellulose.

Keywords: rayon fibers; burning property; dye absorption; water absorption; water drainage



Science Projects for Students Showcase (SS-P-009)

Light phenomenon generator that produces dark field images for use with USB digital microscope

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This device aims to address the limitations of conventional Dark-field microscopes and enhance accessibility to the principles of Dark-field microscopy. The research team developed a more compact microscope model by integrating a USB digital microscope into the design using SketchUp. The model was then 3D printed using PLA material. The device enables focus and light intensity adjustments via a USB digital microscope, with real-time image display and recording on a laptop. The lighting technique, adapted from smartphone-based fluorescence microscopy, utilizes LED to illuminate the sample at an optimal angle. inducing light scattering, generating images with a bright specimen against a dark background. To identify the light intensity that yields the highest contrast, image contrast values from tests at various intensity levels (0.5-5 lux) were analyzed using the OpenCV library with Python programming. The results showed a demonstrated that light intensity significantly affects image contrast, with maximum efficiency observed at an intensity of 3 lux and the highest contrast value of 62.6443 was recorded. These findings suggest that the device has significant potential for improving accessibility to Dark-field microscopy and serves as a practical tool for studying transparent or weakly stained specimens.

Keywords: USB digital microscope; scattering of light; dark-field microscope

Magnifying image device with dual light source fluorescent microscopy technique

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This device is designed for studying the structure and development of embryos. Traditional dark-field microscopes are often heavy and expensive, limiting accessibility. This project aims to develop a compact and affordable alternative device, compatible with smartphones, using 3D printing with PLA filament and adapting fluorescent smartphone microscopy techniques.. The device features dual LED light sources positioned on both sides of the sample slide, generating dark-field effects through light scattering. The microscope integrates a motorized focus adjustment system and a brightness control button to enhance image clarity. It uses polymer lenses (epoxy resin) with 25x, 50x, and 100x magnifications. A smartphone camera is placed beneath the device to capture images. A comparison of contrast values between single and dual light source systems shows significantly higher image resolution with the dual light source, yielding contrast values of 1281829.8 and 2167652.8, respectively. This device expands access to dark-field microscopy for biological research and education, fostering more inclusive scientific opportunities.

Keywords: darkfield; light scattering; contrast value

Science Projects for Students Showcase (SS-P-011)

Non-invasive colorimetric smart paper sensor for urinary glucose detection

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The presence of glucose in urine serves as a critical indicator of metabolic disorders, particularly those associated with impaired kidney function. This study presents the development of a rapid, paper-based analytical device for the preliminary detection of urinary glucose. The assay employs Benedict's reagent in conjunction with a colorimetric detection method. A mixture of 0.08 mol/L Benedict's solution and sodium hydroxide (NaOH) was impregnated onto filter paper, which was then cut into circular test strips and affixed to a plastic film. The detection process involved adding a standard glucose solution (positive control), water (reference), and urine samples onto designated test zones, with triplicate measurements performed for each condition. The strips were subsequently sealed in a zip-lock bag and heated by immersion in water at 90°C for 1 minute. The test zones exhibited a color transition from light blue to pale green and yellow, correlating with glucose concentration. Quantitative analysis based on the standard addition method yielded a detection range of 20–250 mg/dL ($R^2 = 0.9850$), with a repeatability of 1.26% relative standard deviation (RSD) and a limit of detection (LOD) of 18 mg/dL. No statistically significant differences were observed between the proposed method and conventional hospital-based assays. The developed device offers a simple, rapid, and cost-effective alternative for preliminary glucose screening in urine. Furthermore, with the aid of a color reference chart, non-invasive glucose monitoring can be conveniently conducted using household equipment.

Keywords: paper-based sensor; colorimetric detection; urinary glucose screening; non-invasive diagnostics; point-of-care testing

Science Projects for Students Showcase (SS-P-012)

Physicochemical characterization and dye adsorption efficiency of rice hull ash under varied ashing conditions

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Rice hull ash (RHA) is a cost-effective and efficient adsorbent for water purification, with its properties highly dependent on ashing conditions. This study systematically investigates the effects of ashing temperature and atmosphere on the physicochemical characteristics of RHA and its adsorption performance for methylene blue (MB) and Congo red (CR) X-ray diffraction (XRD) analysis confirmed that the silica in all RHA samples exists predominantly in an amorphous form, whereas SEM images demonstrated a porous surface morphology, indicative of a carbonaceous matrix. RHA ashed in an air atmosphere retains carbon, resulting in a mesoporous structure, while the surface area and pore volume of black RHA (BRHA) increase with higher ashing temperatures. Adsorption kinetics followed a pseudo-second-order model, and adsorption isotherms aligned with the Langmuir model, indicating monolayer adsorption of MB. The adsorption capacity correlated linearly with mesopore volume, with white RHA (WRHA) ashed at 450°C and BRHA ashed at 750°C exhibiting the highest MB adsorption capacities ($q_e > 45$ mg g^{-1}). These findings provide valuable insights into optimizing ashing conditions to enhance the adsorptive performance of RHA, contributing to the development of sustainable and low-cost water treatment materials.

Keywords: adsorption; methylene blue; pyrolysis; rice hull ash

Science Projects for Students Showcase (SS-P-013)

Synergistic effect of NiO/CuO nanocomposites for enhanced photocatalytic degradation of methylene blue dye

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Heterojunctions between different semiconductor materials offer a promising strategy to enhance photocatalytic efficiency by improving the separation of photo-induced electrons and holes. In this study, NiO, CuO, and NiO/CuO nanocomposites were successfully synthesized using a simple hydrothermal process. The structural, morphological, and optical properties of the nanocomposites were thoroughly characterized using X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), energy dispersive X-ray (EDX) analysis, transmission electron microscopy (TEM), and UV-visible spectroscopy. The XRD results showed that the NiO/CuO composites possess good crystallinity, with the crystallite size calculated using the Scherrer formula, which was found to be 28 nm. TEM analysis confirmed the formation of the NiO/CuO heterojunctions. The photocatalytic performance of the NiO/CuO nanocomposites was evaluated for methylene blue (MB) dye degradation under 180 min of sunlight exposure. The degradation percentage was 86%, and the rate constant was 0.0065 s^{-1}, demonstrating superior performance compared to the individual oxides. The enhanced photocatalytic activity of the NiO/CuO composite is attributed to the synergistic effect between the two materials, which promotes the creation of defects, reactive species on the surface, and efficient charge carrier separation.

Keywords: heterojunction NiO/CuO; photocatalysis; methylene blue; hydrothermal synthesis; charge carrier separation

Science Projects for Students Showcase (SS-P-014)

Synergistic effects of herbal combinations on health and wellness

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Herbal medicine, rooted in centuries of traditional use, continues to attract scientific interest due to its complex phytochemical composition and potential for multi-target therapeutic action. Increasingly, modern research is turning to combinatorial herbal approaches, which may yield synergistic effects surpassing those of isolated constituents. This study explores the synergistic potential of three widely utilized medicinal plants including turmeric (Curcuma longa), ginger (Zingiber officinale), and garlic (Allium sativum), that noted for their anti-inflammatory, antioxidant, and immunomodulatory properties. To rigorously characterize the phytochemical profiles of these herbs and their combinations, we employed advanced extraction protocols and state-of-the-art analytical techniques, including High-Performance Liquid Chromatography (HPLC) and Gas Chromatography–Mass Spectrometry (GC-MS). Analysis revealed over 25 bioactive compounds, with major constituents including curcumin (21.4 mg/g), 6-gingerol (15.2 mg/g), and allicin derivatives (18.7 mg/g). Notably, in combined formulations, some compounds displayed altered retention times and peak intensities, suggesting potential interactions at the chemical level. The previous report on biological activity was assessed through in vitro assays on human keratinocyte (HaCaT) and mast cell (HMC-1) lines. The herbal combination exhibited a 35% greater inhibition of pro-inflammatory cytokine IL-6 secretion compared to individual extracts ($p < 0.01$). Antibacterial testing against *Staphylococcus aureus* and *Escherichia coli* showed up to 48% enhanced inhibition zones with the combined extract relative to the most potent single herb (garlic). In anti-allergic assays, histamine release was reduced by 62% in combined treatments, compared to 40–45% with individual herbs alone. These results demonstrate significant synergistic interactions among the tested herbs at both the chemical and functional levels, supporting traditional polyherbal practices with robust experimental data. By bridging traditional knowledge with modern analytical and cellular approaches, this research contributes to the rational design of optimized, evidence-based botanical therapeutics. Our accumulation findings offer strong potential for the development of more effective, sustainable, and scientifically validated herbal health products

Keywords: herbal medicine; synergistic effects; turmeric; ginger

Science Projects for Students Showcase (SS-P-015)

Influence of irrigation water quality on the nutritional composition of kale (*Brassica oleracea*) and its implications for human health

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Proper nutrition plays a critical role in preventing common health conditions such as anemia, osteoporosis, and immune system deficiencies. Kale (*Brassica oleracea* var. *sabellica*), known for its dense nutritional profile, is a rich source of essential micronutrients including vitamin C, calcium, and iron. However, the nutritional composition of kale can be influenced by environmental factors, particularly the quality of irrigation water. Water from different sources varies in pH, mineral content, and potential contaminants, all of which can affect plant nutrient uptake. This study investigates the effect of three irrigation water sources, which are including tap water, rainwater, and groundwater with the effect on the nutrient composition of kale. Kale samples were grown under controlled conditions and irrigated with each water type over a four-week period. Post-harvest analysis was conducted using spectrophotometric and titration methods to quantify vitamin C, calcium, and iron content. Preliminary results showed that kale irrigated with rainwater had the highest vitamin C content (up to 62 mg per 100 g fresh weight), while groundwater-irrigated kale exhibited increased calcium levels (up to 200 mg/100 g). Iron concentrations remained relatively stable across all conditions, averaging around 1.5–1.8 mg/100 g. These findings suggest that irrigation water source can significantly influence the nutritional value of kale, with potential implications for both agricultural practices and consumer health. Optimizing irrigation choices could enhance the quality of leafy greens and contribute to more sustainable and nutrient-conscious farming systems.

Keywords: irrigation water quality; nutritional composition; micronutrients; vitamin C

The development of functional jelly by incorporation of lotus stem powder and lotus flower pollen tea with konjac jelly

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The development of functional jelly by incorporation of lotus stem powder and lotus flower pollen tea with konjac jelly**.** This project was conducted with the following objectives: (1) develop a konjac jelly product using lotus rhizome powder, (2) study its physicochemical properties, and (3) evaluate its antioxidant efficiency. The independent variables were lotus rhizome powder, konjac powder, and carrageenan, while the dependent variables were consumer satisfaction, physicochemical properties, and antioxidant activity.

Nine jelly formulas were tested for consumer satisfaction based on taste, color, aroma, and texture by 24 randomly selected participants from Princess Chulabhorn Science High School, Pathum Thani. The most preferred formula, Formula 9, consisted of 1 g of konjac powder, 1 g of carrageenan, 2 g of lotus rhizome powder, 0.01 g of sucralose, and 100 g of lotus flower tea. It received an average satisfaction score of 3.80. The physicochemical analysis showed a lightness (L*) value of 20.33, a red-green value (a*) of 1.70, a yellow-blue value (b*) of 5.47, water activity of 0.98, hardness of 120.05 ± 9.38 N, and antioxidant activity of 81.80%. And when Formula 6, the second most preferred, was compared with a commercial konjac jelly product, it was found to have a similar texture and color, but slightly lower DPPH radical scavenging activity (81.76%).

Keywords: jelly product; lotus rhizome powder; lotus flower pollen tea; antioxidant activity

Science Projects for Students Showcase (SS-P-017)

Extraction and application of natural pigments from Thai and Japanese flowers for sustainable watercolor development

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Natural pigments derived from Thai and Japanese flowers provide eco-friendly alternatives for watercolor. This research aims to develop safe, sustainable, eco-friendly, and hypoallergenic natural watercolors, specifically for individuals with hypersensitive skin and children who cannot use conventional watercolor paints. Additionally, this study seeks to preserve traditional knowledge related to natural pigments. Anthocyanins, water-soluble pigments belonging to the phenolic group, are responsible for the red, purple, and blue hues found in various flowers. Their glycosylated forms enable color changes in response to pH variations due to structural transformations at different acidity levels. [*Bin Tang* **2019**, 107643.] This unique property allows for the creation of natural watercolors that shift in color based on pH changes. The extraction process begins with drying flowers in an oven until completely dehydrated, followed by blending them into a fine powder. The powdered flowers are then mixed with ethanol and left to extract for 2–3 days. After extraction, the mixture is filtered using a vacuum filtration. Subsequently, take it to ethanol evaporation by using distillation apparatus. Then the concentrated pigment is combined with gum Arabic to form a watercolor medium. Test the prepared watercolor and record the observations. The results of these tests are still in progress.

Keywords: extraction; natural pigment; flowers; watercolor; anthocyanin

Development of paper products from sugarcane bagasse coated with extracts anthocyanin from butterfly pea for pH measurement of substances in daily life

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Development of paper products from sugarcane bagasse coated with butterfly pea anthocyanin extract for pH measurement of daily substances by studying the appropriate ratio of sugarcane bagasse and paper pulp for papermaking. Study the properties Physical study of paper thickness, study of solvent type and time affecting the concentration of anthocyanin extract, and test the efficiency of bagasse paper impregnated with anthocyanin from sugarcane flowers. butterfly pea and substances in daily life 1. From the study of the appropriate ratio of bagasse and pulp for paper making, it was found that the ratio of formula 5, bagasse 20 grams, pulp 20 grams, water volume 1600 milliliters, gave the results The best test because the paper sticks together. Durability has the highest value 2. From the results of the study of physical properties in measuring the thickness of paper, it was found that there is consistency with formula 5, the ratio of 20 grams of bagasse, 20 grams of pulp, 1600 grams of water, the thickness of paper. 2.88 cm has not absorbed too much water. 3. The results of the study on the type of solvent that is suitable for anthocyanin extract found that water is the best type of solvent. 4. The results of the study on the time that has an effect Regarding the concentration of anthocyanin extract, it was found that the time of 10 minutes gave no different results. 5. The results of the efficiency test of bagasse paper impregnated with anthocyanin extract, number 8 everyday substances found that the test results with pH gave values close to universal indicator paper.

Keywords: butterfly pea; anthocyanin

Science Projects for Students Showcase (SS-P-019)

The label indicates the freshness of the fish using a film sheet made from crude butterfly pea extract

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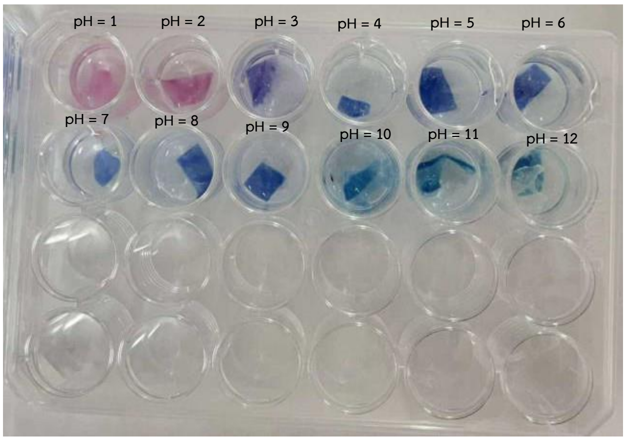
The purpose of this project were to 1) To produce an indicator film from butterfly pea flower extract. 2) To test the effectiveness of the indicator film in changing color when in contact with acidic and basic solutions. 3) To apply the indicator film from butterfly pea flower extract on fish fillets. The project team produced three formulations of the indicator film, which are as follows a Formula 1 mixes cornstarch and water but without glycerol. Formula 2 mixes cornstarch, water and 0.5 grams of glycerol and a formula 3 mixes cornstarch, water and 1 gram of glycerol. The experimental results showed that the formula without glycerol had lower film formation efficiency compared to the other two formulations. The formula with 1 gram of glycerol was found to be the most effective and producing a flexible film because glycerol is a plasticizer and making the film more flexible by interacting with the starch molecules. it helps form a polymer. The observation of the color change in pH values used to test all three formulas showed good efficiency, as the color could change according to the pH value when no film was formed. Furthermore, the produced film can change color according to pH when it comes into water or vapor. Additionally, the performance of the film indicates the freshness of fish meat well within 7 days changing from blue to green. The fish meat developed a foul odor and slimy, fishy mucus, indicating that the indicator film can show the freshness of the fish. This is because the spoilage of fish releases ammonia gas which has a pH of 11 within the basic range.

Keywords: butterfly pea flower; film indicator; freshness of the fish



Science Projects for Students Showcase (SS-P-020)

The study of the solubility properties of gases using a small-scale chemistry on the phenomenon of ocean acidification

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The purpose of this project were to 1) To explain the phenomenon of ocean acidification. 2) To investigate the factors that affect the solubility of substances in the gaseous state. The Small-scale chemistry to study the ocean acidification consists of investigating the effect of temperature on the solubility of carbon dioxide gas. it was found that when the amount of calcium carbonate is increased, it results in a greater production of carbon dioxide gas and when water at a temperature of 20 degrees celsius (cold water) takes less time to change the color of the universal indicator from green pH 7 to yellow pH 6. Therefore, carbon dioxide gas dissolves better in water at this temperature than in water at 70 degrees celsius. The project team can explain the phenomenon of ocean acidification by observing the color change of the universal indicator. This experiment raises awareness of the impact of ocean acidification, which leads to a decrease in the number of marine species with hard outer shells, and causes the loss of habitats for various marine organisms. It fosters a scientific attitude towards reducing activities that contribute to the release of carbon dioxide gas.

Keywords: affect solubility; carbon dioxide gas; eggshells

Science Projects for Students Showcase (SS-P-021)

Development of a smartphone-based colorimetric method for the determination of phenolphthalein

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Phenolphthalein (PP) is an indicator used in acid-base titrations and exhibits distinct color variations within its active pH range, which are directly proportional to the concentration of the solution. In this study, a smartphone-based colorimetric method was developed for the determination of phenolphthalein, which is restricted due to its carcinogenic properties [*J. Chem. Edu.* **2008**, *85*(8), 1152.]. Using images captured with a smartphone, RGB (red-green-blue) color scale values were determined through a software application. A relationship was established between the RGB data of colored samples and analyte concentrations [*Measurement* **2021**, *171*, 108829.]. Besides, smartphones offer numerous advantages, including widespread availability, easy accessibility, and compatibility with various applications. With today's technology, smartphones are preferred due to their superior imaging quality, high-speed processors, and the widespread use of mobile applications (APPs). Considering these advantages, images in this study were recorded using a smartphone. The developed colorimetric method is a simple, low-cost, and environmentally friendly approach for identifying potentially harmful compounds. To test the applicability of the developed method, recovery studies were conducted in tap water. The recovery results obtained close to 100% proved the applicability and accuracy of the developed method in real samples.

Keywords: indicator; phenolphthalein; smartphone-based colorimetry; tap water

Science Projects for Students Showcase (SS-P-022)

First-row transition metal ions and porphyrin derivatives: Exploring electronic and catalytic implications

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Porphyrins and metalloporphyrins are heterocyclic macrocyclic compounds in which transition metal ions are typically coordinated within the central cavity of the porphyrin ring. In this study, free-base porphyrins were synthesized via a condensation reaction between pyrrole and various aldehydes in propionic acid, following the Adler-Longo method. Subsequent metallation was achieved through refluxing in dimethylformamide (DMF) with selected metal salts, followed by purification. The synthesized compounds were characterized using elemental analysis and mass spectrometry, which confirmed their compositional agreement with theoretical values. Fourier-transform infrared (FTIR) spectroscopy was employed to identify key functional groups, while ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectroscopy confirmed the structural integrity of the synthesized porphyrins. Ultraviolet-visible (UV-Vis) and fluorescence spectroscopies were used to investigate their electronic properties. The absorption spectra of free-base porphyrins exhibited an intense Soret band (412–417 nm) and four characteristic Q-bands (512–654 nm). Upon metallation, the increased symmetry of the macrocycle resulted in the simplification of the Q-band pattern, reducing to one to three absorption bands. Fluorescence measurements of free-base porphyrins revealed a single emission peak in the 647–654 nm range. Metallation led to an enhancement in fluorescence intensity, indicating an influence of the coordinated metal ion on the electronic properties of the porphyrin core. The thermal stability and phase transitions of the synthesized porphyrins were investigated in the 300–950 K range. Among the free-base porphyrins, TPP 1 exhibited the lowest thermal stability, whereas CoTMPP demonstrated the highest stability, with a decomposition temperature of 733.4 K. These findings provide valuable insights into the structural, electronic, and thermal properties of porphyrins and their metallated derivatives, which are relevant for potential applications in catalysis, photodynamic therapy, and materials science.

Keywords: metalloporphyrin; TGA; NMR; mass spectrometry

Science Projects for Students Showcase (SS-P-023)

Strengthening chemical security for sustainable nanotechnology in environmental research

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This study examines the dual-use nature of chemicals in academic research, emphasizing the balance between scientific advancements and potential risks to human health and the environment. A key focus is addressing chemical security gaps within the University's Department of Chemistry, particularly in senior research projects. Over the past five years, a dedicated chemistry lecturer has led chemical security training for academic and industrial practitioners while conducting research on heavy metal detection and analytical methods. A case study involving ammonia gel for detecting nickel(II) and cobalt(III) in wastewater highlights the importance of safe handling protocols. Additionally, the study explores the synthesis of gold nanoparticles using citric acid from citrus fruits, demonstrating their potential for removing nickel from aqueous solutions. Characterization techniques such as FT-IR, TEM, SEM, XRD, and SAED confirm the efficiency of these nanoparticles. This approach integrates chemical security training with sustainable nanotechnology applications, fostering a safer academic research environment. The findings underscore the need for enhanced safety protocols, environmental responsibility, and hands-on STEM education. By aligning research practices with Sustainable Development Goals (SDGs), this study promotes responsible chemical management and innovative solutions for environmental challenges.

Keywords: ionic precipitation; anions and cations; precipitate formation

Science Projects for Students Showcase (SS-P-024)

Upcycling oyster shell waste for biodiesel production

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This study investigates the utilization of waste oyster shells as a sustainable source of calcium oxide catalysts for biodiesel production through the transesterification of palm oil. A key innovation lies in the pelletization of the catalyst, enhancing separation, handling, and reusability within the biodiesel reactor. Waste shells were calcined at 900°C for 5 hours, converting calcium carbonate into calcium oxide. The catalyst was characterized using X-ray Diffraction (XRD), Thermo-Gravimetric Analysis (TGA), Fourier Transform Infrared Spectroscopy (FT-IR), and Scanning Electron Microscopy (SEM). Under optimized reaction conditions (5-hour reaction time, 10% catalyst loading, 80°C temperature, 3:1 methanol-to-oil ratio), biodiesel conversion exceeded 98%. The reusability of the catalyst was further assessed, maintaining yields above 80% over ten reaction cycles, demonstrating its durability and cost-effectiveness for large-scale biodiesel production. These findings highlight the potential of waste-derived catalysts in promoting sustainable and efficient biofuel synthesis while aligning with circular economy principles and renewable energy goals.

Keywords: oyster shell; calcium oxide; biodiesel

Science Projects for Students Showcase (SS-P-025)

Innovative photo-electrocatalytic cells for sterilizing PVC medical devices

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Klebsiella pneumoniae is a bacterium that resides in the human body and can become pathogenic under conditions of weakened immunity. Hospital-acquired infections are a common issue, these infections can be transmitted through physical contact and especially through medical devices such as urinary catheters and endotracheal tubes made of PVC plastic, which may degrade during cleaning or sterilization processes. This study focuses on developing sterilization technology using photo-electrocatalysis, employing electrodes coated with ZnO and TiO_2 to enhance the production of hypochlorous acid (HClO) and hypochlorite ions (ClO^-), which have strong antimicrobial properties. The experiments included the light-activated catalytic reactions across both visible and UV light spectrums to study the reactivity of each semiconductors based on their absorbance and examined their effects on the physical and chemical properties of PVC using techniques such as FTIR, DSC, and tensile testing. The experiment results appeared as the innovation can effectively sterilize *Klebsiella pneumoniae* at a concentration of 10^6 CFU/mL in 80 minutes and decrease the detachment of Phthalates to the rate that cannot affect humans and harm PVC's properties.

Keywords: *Klebsiella pneumoniae*; polyvinyl chloride; photo-electrocatalysis

Science Projects for Students Showcase (SS-P-026)

Production of watercolors from plants

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The project titled *"Production of Watercolors from Plants"* investigates the development of environmentally friendly watercolors using natural pigments extracted from plants. The primary objectives were: (1) to study the extraction and formulation of watercolors from three pigment-rich plant species; ***Clitoria ternatea*** (butterfly pea), ***Hibiscus sabdariffa*** (roselle), and ***Curcuma longa*** (turmeric); (2) to examine the effects of two natural additives, glycerin and gum arabic, on the physical properties of the paint; and (3) to evaluate the performance of these natural watercolors in comparison to three commercial synthetic brands.

Plant pigment extraction was carried out via aqueous boiling at 90–100°C for 15–30 minutes, yielding an average of 10–15 mL of concentrated dye per 50 g of plant material. The extracted pigments were then mixed with 5%, 10%, and 15% concentrations of glycerin and gum arabic to assess differences in texture, spreadability, and drying time. Color intensity was measured using a colorimeter, with absorbance values ranging from 0.25–0.68 AU, indicating moderate to strong pigment presence. Lightfastness tests under direct sunlight for 72 hours showed a 10–35% reduction in color intensity, depending on the pigment type and binder ratio. Comparative analysis with commercial watercolors included evaluations of color vibrancy, drying time, and paper adhesion. Although synthetic watercolors outperformed natural ones in terms of color permanence and saturation, plant-based alternatives demonstrated acceptable performance levels for educational and hobbyist use, while also offering advantages such as non-toxicity and biodegradability. This study supports the feasibility of plant-based pigments as sustainable coloring agents and highlights their potential applications in eco-conscious art and education.

Keywords: natural pigments; plant-based watercolor; *Clitoria ternatea*; *Hibiscus sabdariffa*; *Curcuma longa*

Science Projects for Students Showcase (SS-P-027)

Extraction and refinement of microcrystalline cellulose from rice straw via physical and chemical modifications

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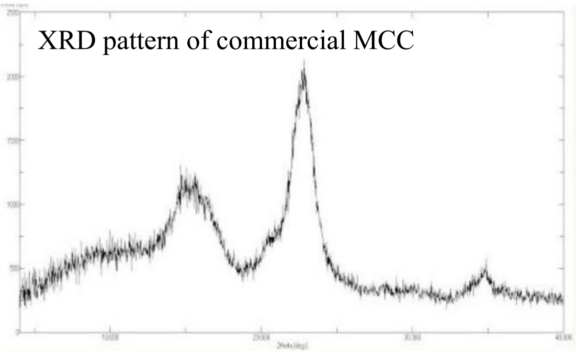
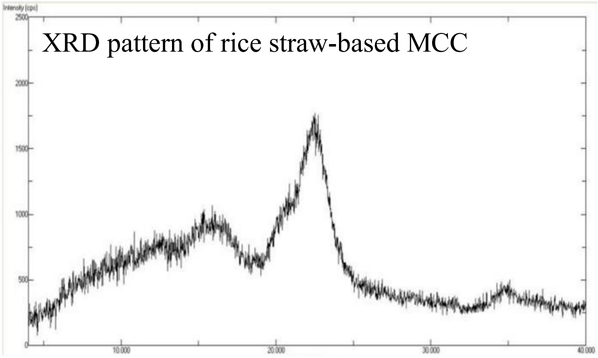
This study aimed to develop an eco-friendly tablet excipient using microcrystalline cellulose (MCC) extracted from rice straw which is a sustainable and cost-effective cellulose source. MCC is essential in tablet production, serving as a diluent, binder and glidant to enhance integrity and drug uniformity. The extraction process involved alkali treatment (NaOH), bleaching (H_2O_2), and acid hydrolysis (HCl) to purify cellulose and improve its crystallinity. Fourier-transform infrared spectroscopy (FT-IR) confirmed successful lignin removal, ensuring a purified cellulose structure suitable for MCC production. Evaluation of tablet compressed from isolated MCC demonstrated promising results. Hardness testing yielded an average of 4.85 kPa, indicating effective binding properties, while weight uniformity analysis showed consistent tablet weights, ensuring good flowability. The analysis by a powder X-ray diffractometer confirmed that the MCC obtained from rice straw is in the microcrystalline form (MCC), similar to commercial MCC. These findings suggest that rice straw-based MCC can serve as a high-performance, sustainable alternative to conventional excipients in pharmaceuticals. Its ability to enhance tablet properties, coupled with its environmental benefits, supports its viability for commercial applications.

Keywords: microcrystalline cellulose; alpha cellulose; rice straw; pharmaceutical excipient



XRD pattern of commercial MCC



XRD pattern of rice straw-based MCC

Science Projects for Students Showcase (SS-P-028)

Hydroxyapatite/tri-calcium phosphate (HAp/TCP) 3D porous scaffold composites coated with carboxymethyl cellulose

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This study used hydroxyapatite (HAp) and tri-calcium phosphate (TCP) to fabricate 3D porous bone scaffolds via the Foam Replica method with polyurethane (PU) as a template. The TCP concentration (0, 5, 10, 15, and 20 wt%) was varied to study its effect on scaffold characteristics. TCP, which possesses calcium properties that foster biocompatibility and promote cell growth, was incorporated to enhance ion attraction and support tissue regeneration. The results showed that the 20% TCP scaffold had the most suitable post-shrinkage (41.76%) and post-sintering density increase (31.63%), which is the lowest among all samples. However, higher ratio of HAp in composites led to a greater shrinkage and density. To improve, carboxymethyl cellulose (CMC) was applied as a coating on the HAp/TCP scaffolds using sonication and vacuum methods, with CMC concentrations of 1% and 1.5% (w/v). The addition of CMC significantly improved the mechanical strength, addressing the low pressure-bearing capacity of HAp/TCP scaffolds. The compressive strength, measured using a universal testing machine (UTM), showed notable improvement, with 1% and 1.5% CMC-coated scaffolds exhibiting 1.4–4.6× and 1–3.5× increases, respectively. Additionally, CMC-coated scaffolds exhibited a slight reduction in pore size; however, the pores remained within the optimal range of 200–400 µm.

Keywords: bone scaffold; hydroxyapatite; tri-calcium phosphate; carboxymethyl cellulose

Science Projects for Students Showcase (SS-P-029)

Prototype electrolysis device for rust removal from watch screws

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Rust commonly forms on wristwatch screws because of exposure to sweat, water, and humidity, which can compromise their integrity and lifespan. While traditional rust removal techniques like chemical treatments and mechanical abrasion exist, they risk damaging the metal or using harmful chemicals. Electrolysis, which harnesses the power of ions to break down iron oxide, offers an alternative approach to rust removal. This study aimed to: 1) investigate optimal conditions for rust removal from metal, and 2) develop and test a rust-cleaning device for watch screws using electrolysis. It comprised two experiments. The first examined the effects of different electrolytes and their concentrations. Results showed that Na_2CO_3 proved to be the most effective electrolyte, with an optimal 0.008 M concentration at 9 V. This condition had a higher percentage of rust removed than a control by 2.50 times. The second experiment involved designing and testing a prototype cleaning device based on these conditions. The device was used to treatment rusted watch screws for a duration of 10 minutes. Effectiveness was evaluated by measuring rust weight before and after cleaning, the reusability of the solution, and user satisfaction by a hedonic 5-point scale. Findings indicated that the developed device efficiently removed rust, the number of successful cleaning cycles using the same solution is 6 times more than that control for 1.5 fold, and users expressed a high level of satisfaction ($\overline{x}$= 4.07).

Keywords: small scale; electrolysis; rust removal; electrolyte solution

Science Projects for Students Showcase (SS-P-030)

Development of a field test kit and smartphone-based application for hexavalent chromium detection in water

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Chromium contamination in soil and water represents a significant environmental and public health concern, primarily due to the high solubility and carcinogenicity of hexavalent chromium (Cr^{6+}). Conventional Cr(VI) detection requires laboratory-based analysis by trained personnel, making it time-consuming and costly. This study aimed to develop a field-deployable test kit and a smartphone-based application for Cr(VI) detection in wastewater. The kit utilized chelating and colorimetric agents—EDTA, semicarbazide hydrochloride, and 1,5-diphenylcarbazide. Optimal pH and reaction time were determined by reducing Cr(VI) to Cr(III) using ascorbic acid, followed by spectrophotometric analysis. Method validation was performed using synthetic and real wastewater samples, with percent recovery (%Recovery) evaluated.

Results showed that Cr(III) formed a stable complex with semicarbazide hydrochloride within 20 minutes using 10 mL of 1000 ppm Cr(III) and 2 mL of 1.0% w/v reagent. Interference from calcium and sodium ions was negligible. A linear calibration curve (R^2 = 0.997) demonstrated high precision, and the mobile application yielded recovery rates close to 100%, indicating its potential as a rapid, cost-effective, and eco-friendly tool for on-site Cr(VI) detection.

Keywords: hexavalent chromium; field test kit; smartphone application

Science Projects for Students Showcase (SS-P-031)

Development of a hydrogel patch from pomelo peel for inhibiting *Staphylococcus aureus* infection found in diabetic foot ulcers

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Diabetes is increasing among the elderly, who are at risk of complications such as diabetic wounds infected with *Staphylococcus aureus*. Studies have shown that flavonoids from pomelo peel have antioxidant and antibacterial properties, helping to inhibit the growth of *S.aureus* and having potential in the treatment of diabetic wounds. This study aims to evaluate the effectiveness of hydrogel patches made from pomelo peel extract in inhibiting *S.aureus* in diabetic foot wounds. The pomelo peel was extracted using 95% ethanol, followed by the analysis of the active compounds and biological activities. The inhibition of the bacteria was tested using the disc diffusion method. The results showed that the extract contained an average flavonoid content of 26.57 ± 8.59 mg QE/g, and the antioxidant activity had an IC_{50} value of 0.154 mg/mL. The highest inhibition zone was 1.53 ± 0.12 cm. The extract was then developed into hydrogel patches with two different production ratios 25:2:2:2:1 %w/v and 30:2:3:3:2 %w/v (PVA: glycerol: sodium alginate: glutaraldehyde: extract). Based on the evaluation of their properties, the hydrogel patch with a ratio of 30:2:3:3:2 exhibited the best properties, including water absorption of 250%, extract release of 65% after 24 hours, skin adhesion force of 1.2 N, and a pH value of 6.5, demonstrating the safety and suitability for use on human skin.

Keywords: pomelo peel; flavonoid extract; *Staphylococcus aureus*; hydrogel patch

Acceleration of molting in black crabs with mulberry leaf extract

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Soft-shell crab is a high-demand fishery product, but traditional molting acceleration methods involving cutting claws and legs harm crabs. This research investigated using crude mulberry leaf extract as a safe alternative to accelerate black crab molting. The study involved extracting substances from mulberry leaves using 60% ethanol, and analyzing the phenolic content. Black crabs weighing 100-150 g were individually raised in baskets and fed with food containing various concentrations of the extract (0-30 mg per 100 g) for three weeks. The results showed that the extract contained 24.44-24.71mg gallic acid per 100 g. The optimal concentration was 15 mg per 100 g of food which reduced molting time from 10.2 to 5.8 days, increased weight by 12.5% compared to 9.8% in the control group, and improved Feed Conversion Ratio (FCR) from 2.3 to 1.8. These findings align with previous research showing that plant phenolic compounds affect aquatic animal development, possibly by stimulating the production of the ecdysone hormone in crustacean molting. The mulberry leaf extract offers a safer way to reduce cultivation time and increase productivity. It minimizes the risks of death to crabs while enhancing the sustainability of soft-shell crab farming, addressing both economic and animal welfare concerns.

Keywords: soft-shell crab; molting acceleration; mulberry leaves; crude extract from mulberry leaves

Science Projects for Students Showcase (SS-P-033)

Development of a synthesis process for metal-organic framework materials using organic ligands derived from plastic waste degradation

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Metal-Organic Frameworks (MOFs) are nanocomposites with high surface area, porosity, low density, and excellent thermal stability, making them ideal for applications such as gas filtration and catalysis. MOFs are typically formed through the chemical bonding of metal ions with organic ligands, creating a network-like structure. However, the organic ligands used in MOF synthesis are often derived from costly laboratory-synthesized compounds. This study aims to repurpose polyethylene terephthalate (PET) plastic waste by depolymerizing it through alkaline and acidic hydrolysis into terephthalic acid (TPA), which can then be used as a ligand in MOF synthesis. The depolymerization process yielded high-purity TPA, with a yield of up to 62.5%. The extracted TPA was then used to synthesize MOFs with copper nitrate trihydrate via a solvothermal process at different molar ratios (Cu(II): TPA) of 2:1, 1:1, and 1:2. The properties of the Cu-TPA MOFs were analyzed using FT-IR spectroscopy, X-ray diffraction and thermogravimetric analysis (TGA). The results showed that the 1:2 Cu-TPA ratio produced the highest purity and was most suitable for further applications. This study provides a cost-effective approach to producing high-value MOFs from plastic waste, offering potential applications in various fields.

Keywords: polyethylene terephthalate; metal-organic frameworks; organic ligands

Development of a field test kit for ammonia and nitrate determination in water using colorimetric analysis via mobile application

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Ammonia and nitrate are key indicators of water pollution, commonly linked to fertilizers, domestic wastewater, and organic matter. This study presents a low-cost, rapid, and reliable field test kit for detecting ammonia and nitrate in surface water. Samples were collected from natural water sources and general wastewater to evaluate performance. Ammonia detection relies on a redox reaction between ammonia and sodium hypochlorite, catalyzed by sodium nitroprusside. Under optimized conditions, 1.0 mL of water is mixed with 0.05 g of sodium hypochlorite and five drops of sodium nitroprusside, then left to react for 15 minutes to form a green complex. Nitrate detection involves reducing nitrate to nitrite, followed by a reaction with sulfanilic acid and α-naphthylamine to form a pink-red azo dye. The procedure uses 10.0 mL of water, 0.5 mL of sulfanilic acid, and 0.12 g of a reagent mixture containing manganese sulfate, zinc powder, and EDTA, with a 20-minute reaction time. A mobile application, developed in JavaScript, converts RGB values into concentrations using calibration curves. Detection ranges are 0.5–20.0 mg/L for ammonia and 1.0–50.0 mg/L for nitrate, with RSD below 10%. LODs were 0.3 mg/L for ammonia and 0.1 mg/L for nitrate. A paired t-test showed no significant difference from UV-Vis spectrophotometry.

Keywords: ammonia detection; nitrate detection; colorimetric test kit; mobile application; water quality analysis

Science Projects for Students Showcase (SS-P-035)

Microencapsulation of red kidney bean extract: α-Glucosidase inhibition, antioxidant activity, and potential for functional food development

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This study explores the potential of crude extract from red kidney beans (*Phaseolus vulgaris*), which are naturally rich in flavonoids and anthocyanins, to inhibit α-glucosidase an enzyme that breaks down complex carbohydrates into simple sugars in the small intestine. Inhibiting this enzyme may help control blood sugar levels after meals. The extract was obtained by maceration with methanol at room temperature, followed by hexane partitioning, resulting in a yield of 1.72% (w/w).

The extract was then microencapsulated using spray drying with 11% w/v hydrolyzed protein as the wall material. The process was carried out under optimized conditions: inlet temperature of 190°C, outlet temperature of 76°C, and rotary atomizer speed of 450 rpm. The microcapsules showed improved solubility and exhibited α-glucosidase inhibitory activity of up to 31.07%. Triacylglycerols (TAGs), identified as key active compounds, are known to help lower blood sugar. Antioxidant analysis revealed DPPH radical scavenging activity of 35.72 mmol TE/Kg and an average total phenolic content of 1624.8 mg GAE/Kg. Storage at 4°C in aluminum foil pouches was most effective in preserving bioactive compounds. Microencapsulated red kidney bean extract shows improved solubility, stability, and bioactivity, supporting its potential as a natural ingredient for dietary blood glucose control.

Keywords: α-glucosidase inhibition; red kidney bean extract; microencapsulation

Wound healing gel formulated with jellyfish-derived collagen and crude *Centella asiatica* extract

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Wounds from accidents often heal slowly and are prone to inflammation, especially in patients with limited access to wound care products due to their high cost. This study aims to develop a wound healing gel formulated with jellyfish-derived collagen and crude *Centella asiatica* extract. These natural ingredients possess antimicrobial, anti-inflammatory, moisturizing, and tissue-regenerating properties. Initially, *Centella asiatica* extract was obtained by maceration in 70% ethanol. Antioxidant activity was assessed using the DPPH assay, yielding an IC_{50} value of 167.54 µg/mL. Additionally, coagulation tests demonstrated that extract concentrations ranging from 0.0814 to 1 mg/mL enhanced blood clotting. Jellyfish (*Lobonema smithii*) collagen was extracted using 0.6 M acetic acid and quantified *via* the sirius red assay, revealing a collagen concentration of 1.75 ± 0.12 mg/mL or 65.4 ± 3.2% of the total sample. The gel formulation was developed using polyvinyl alcohol (PVA), ensuring rapid film formation, flexibility, durability, and ease of application. Experimental results indicate that this jellyfish collagen-*Centella asiatica* gel has significant potential for wound treatment. Furthermore, utilizing jellyfish and *Centella asiatica*—both of which have become overabundant in aquatic ecosystems—offers an eco-friendly solution to environmental imbalances. This innovation could be further developed for commercial applications, providing a sustainable and cost-effective alternative for wound care.

Keywords: *Centella asiatica*; *Lobonema smithii*; polyvinyl alcohol; collagen

Science Projects for Students Showcase (SS-P-037)

Development of soft cellulose splints from pineapple leaf fibers

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A soft splint is a medical device used to stabilize bones or joints, supporting and protecting injured areas to alleviate pain. Most soft splints are made of plastic, which is difficult to break down and causes environmental pollution. These splints are often single-use, contributing to global warming. Pineapple is a popular crop in Thailand because it is resilient to different environments. Only the fruit is used, while the leaves are typically discarded. This project aims to develop soft cellulose splints from pineapple leaf fibers. It studies the molding and effectiveness of cellulose splints made from pineapple leaf fibers mixed with pectin and sodium alginate. The tests measured tensile and compressive strength using a Digital Force Gauge and thickness using a digital micrometer at 9 points, then averaged the results. The optimal ratio for the splints was found to be 15:0.5:2:1 (pineapple leaf cellulose : pectin : sodium alginate : glycerol), with a maximum tensile strength of 10.1 N, compressive strength of 16.1 N, and thickness of 1.77 mm. Therefore, it is possible to create biodegradable plastic splints from pineapple leaf cellulose mixed with pectin and sodium alginate.

Keywords: soft splint; biodegradable plastic; pineapple leaf fibers; molding

Science Projects for Students Showcase (SS-P-038)

Development of a portable colorimetric test kit for glufosinate-ammonium detection using potassium permanganate reaction and micro:bit integration

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Glufosinate ammonium is a widely used herbicide that can contaminate water sources and pose environmental and health risks. However, field detection methods are often expensive, complex, and dependent on laboratory equipment. This study presents a portable, affordable, and user-friendly colorimetric test kit using a redox reaction between potassium permanganate and glufosinate ammonium, which produces a visible color change from purple to pale yellow at pH 3–4. A Micro: bit microcontroller with a digital color sensor converts RGB values into concentration data using a calibration curve. To operate, users add 10.00 mL of sample into a vial, introduce 0.50 mL of sulfuric acid (0.06 mol/L) and 5 mg of $KMnO_4$, stir for 30 seconds, and allow the color to stabilize before measurement. The system accurately detects glufosinate-ammonium in the 1–1,000 ppm range, with a detection limit of 0.5 ppm and an R^2 value exceeding 0.98. High precision (RSD < 5%) and good reproducibility were observed. Interference studies with Fe^{3+}, humic acid, glyphosate, and ascorbic acid showed minimal impact, except for ascorbic acid, which was mitigated by pretreatment or EDTA. Integrating redox chemistry with digital sensing provides a practical, on-site solution for herbicide monitoring in environmental settings.

Keywords: glufosinate-ammonium; colorimetric detection; potassium permanganate; micro:bit sensor; environmental monitoring

The development of semi-instant rice to enhance antioxidant content from Latos seaweed (*Caulerpa sertulaeioides*) and native rice from Satun

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Latos seaweed is a type of plant found along the Andaman coast, with a significant presence in Satun province. They are rich in protein and antioxidants and have high nutritional benefits which can enhance the nutritional value of white rice when added. In this study, Latos seaweed was therefore tested for its antioxidant properties before being used to coat three types of rice: Alhamdulillah rice, a native rice from Satun, Jasmine rice, which is popular among Thais, and Japanese rice, which has long been paired with seaweed. The test found that the seaweed contained antioxidants with a high inhibition value and an IC_{50} value of 1.89 μg/mL.When coated onto white rice and subsequently tested for consumer acceptance, it was found that Alhamdulillah rice retained the appearance of regular white rice, without typical seaweed odor while the taste and smell of the rice remained unchanged, with a slight seaweed taste and moderate, tender texture which makes it the most accepted by consumers. The nutritional analysis showed that 150 grams of the product contained 4 grams of protein, 39 grams of carbohydrates, 45 milligrams of sodium, and 60 milligrams of potassium, indicating that semi-instant rice coated with Latos seaweed enhances the benefits of protein and antioxidants and contains low sodium while offering convenience and speed in consumption which suits today's consumer lifestyle.

Keywords: semi-instant rice; *Caulerpa sertulaeioides*; Latos seaweed; antioxidant

Science Projects for Students Showcase (SS-P-040)

Development of a paper-based for the measurement of ferrous metal ions in water using tannin extracts

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Clean water availability is decreasing due to pollution from human activities, especially chemical spills that lead to contamination with iron and heavy metals beyond safety standards. These pollutants pose serious risks to living organisms. Traditional methods for detecting iron in water are often costly and time-consuming. This project aims to develop a paper-based colorimetric sensor using tannin extract from mangrove bark as a reagent for iron ion detection. The sensor provides a low-cost, simple, and convenient alternative for preliminary water quality testing.The sensing mechanism is based on the reaction between iron ions (Fe^{3+}) and the polyphenolic groups in tannins, forming a blue-black iron–tannin complex. This reaction causes a visible color change on the paper strip, with darker shades indicating higher iron concentrations. The experiment involved extracting tannin from mangrove bark and optimizing key conditions, including tannin concentration and reaction time. Tannin was successfully extracted at a yield of 1.7 mg/L. The optimal condition for color development was found to be 0.5 g of tannin dissolved in 100 mL of ethanol with a 2-minute reaction time.The developed sensor demonstrated clear, concentration-dependent color changes, allowing for rapid and qualitative detection of iron ions in water.

Keywords: clean water; iron detection; tannin extract; paper-based sensor; colorimetric analysis

Science Projects for Students Showcase (SS-P-041)

Biotransformation of insoluble heavy metal compounds by isolated fungi from Pilok mine, Kanchanaburi, Thailand

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Fungi can be found anywhere, including places that are contaminated with heavy metals. This project aims to study mechanics of fungi in biotransformation, including solubilizing and immobilizing insoluble heavy metal compounds. These metals include lead (II) oxide (PbO), copper (II) oxide (CuO), zinc (II) oxide (ZnO), and molybdenum (VI) oxide (MoO_3). The heavy metals are from Pilok mine, Kanchanaburi, Thailand to isolate the fungi which will be plated on Potato Dextrose Agar (PDA) medium with 0.5% (w/v) of heavy metal compounds. S1 and S2 (names used in this project) show significant performance with larger clear zone diameters. The fungi are separated into liquid PDA medium with their respective heavy metal compounds, pH profile is measured which had downward trend. This confirms that fungi is capable of producing acids to immobilize the heavy metals. The crystals from the colony are then purified and analyzed using x-ray diffraction (XRD), they are in the form of oxalates (eg. CuC_2O_4, Monoclinic) and oxalate hydrates (eg. $PbC_2O_4 \cdot 2H_2O$, Triclinic) which were the more stable heavy metal compounds than oxides. This indicates that fungi can detoxify the areas that are polluted with heavy metals by changing the form of metals into less toxic forms proved by XRD.

Keywords: biotransformation; fungi; heavy metal; immobilizing; solubilizing

Science Projects for Students Showcase (SS-P-042)

The study and synthesis of superparamagnetic solution from *Celastrus paniculatus* Willd. for microplastic separation

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This study aims to develop a superparamagnetic solution from *Celastrus paniculatus* seed oil for separating four types of microplastics, including polypropylene, polystyrene, low-density polyethylene, and polyethylene terephthalate glycol from water sources.

The results showed optimal conditions for extracting oil using a hydraulic press at a pressing speed of 20 rpm, yielding the highest oil content at 32.11% by weight. Chitosan-coated Fe_3O_4 nanoparticles were then synthesized using co-precipitation and cross-linking methods. FTIR analysis confirmed the presence of bonds corresponding to chitosan-coated Fe_3O_4 nanoparticles. The 10% w/v nanoparticle oil solution had a viscosity of 50–500 mPa·s, which was suitable for microplastic separation and exhibited excellent superparamagnetic properties.

Microplastic separation tests showed a removal efficiency of over 87.7%, reaching up to 91.7%, depending on the microplastic type used in the experiments. Microplastic separation was carried out using magnetic force, where a magnet was used to extract the oil containing microplastic particles from water. For real-world implementation, water samples were collected from ten sites in Mueang District, Chiang Mai. The synthesized superparamagnetic solution achieved 100% removal efficiency, demonstrating the effectiveness and practical applicability of *Celastrus paniculatus* seed oil for microplastic separation from water sources.

Keywords: microplastic separation; superparamagnetic; *Celastrus paniculatus* Willd.

Science Projects for Students Showcase (SS-P-043)

Magnetic fields form cylindrical permanent magnets

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This project was to measure magnetic fields from a cylindrical permanent magnet, a high-power neodymium (NdFeB) magnet that provides high magnetic field intensity but light weight magnet. Magnetic field lines from the magnets were presented by using iron powder. The magnetic fields were measured with a Tesla meter with a resolution of one decimal place. The cylindrical permanent magnets to be tested consist of five sets of magnets: 1) one cylindrical magnet, 2) two cylindrical magnets, 3) three cylindrical magnets, 4) four cylindrical magnets, and 5) five cylindrical magnets. In the experiment, the magnetic fields at the surface of a cylindrical permanent magnet were measured at different radial distances. The magnetic field decreases as the radial distance increases. When measuring the magnetic field at the center surface of a cylindrical permanent magnet, it was found that the magnetic field increases as the number of magnets increases, but not linearly, possibly due to the cancellation of the magnetic field from the other magnets. In application, we can select the magnets that are suitable for various applications, such as measuring blood flow rate in blood vessels, controlling drug delivery devices, and performing surgery in the abdominal cavity where magnetic surgical devices are controlled, etc.

Keywords: cylindrical permanent magnet; magnetic fields; neodymium magnet

Effect of coconut fiber filler on mechanical & physical properties of PBS bioplastic

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This research investigated the effects of adding chemically-treated coconut fibers as fillers on the tensile strength, impact resistance, hardness, and density of polybutylene succinate (PBS) composites. Coconut fibers with varying contents of 0, 5, 10, 15, and 20 pph were mixed with PBS through a twin-screw extrusion process and molded into test specimens using a hot compression molding. Properties evaluated in this work included tensile strength, impact resistance, hardness, density, and fiber alignment in PBS bioplastics. The results showed that hardness (Shore D) and density for all samples were in the ranges of 66-68 and 1.20-1.31 g/cm^3, respectively. Furthermore, incorporating 10-15 pph of coconut fibers to PBS bioplastic increased the tensile modulus and impact resistance. However, tensile strength and elongation at break generally decreased with increasing fiber content. The results also indicated that fiber alignment exhibited negligible impacts on PBS properties. Overall, the findings suggested that incorporating chemically-treated coconut fibers improved mechanical properties, specifically toughness and strength, of PBS bioplastics. This approach not only promoted the use of biodegradable plastics but also added value to agricultural waste, as well as contributed to environmental sustainability.

Keywords: bioplastic; coconut fiber; mechanical properties; polybutylene succinate

Science Projects for Students Showcase (SS-P-045)

Developing a small-scale spectrophotometer for high school chemistry experiments

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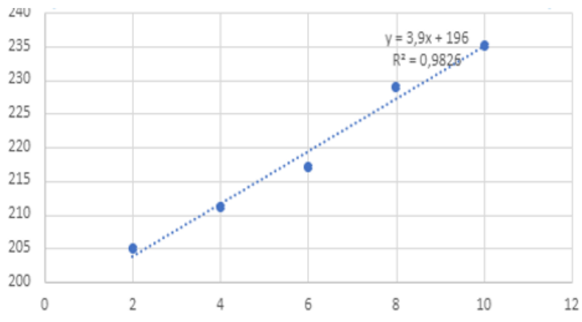
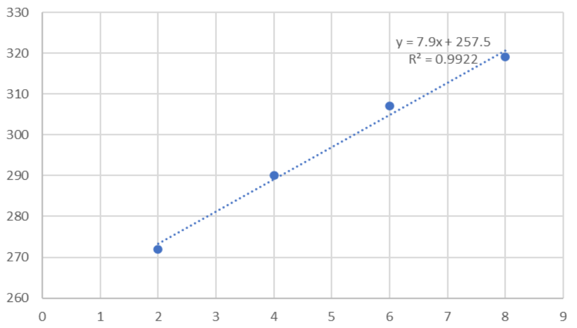
Teaching chemistry in Vietnam emphasizes competency development, particularly in the field of chemistry, where practical application is key to understanding concepts. Spectrophotometry experiments, even on a small scale, can significantly enhance learning, such as determining unknown concentrations. This research focuses on developing an affordable and effective spectrophotometer tailored for high school chemistry experiments, addressing the limitations of costly and complex commercial instruments often unsuitable for small-scale laboratory setups. The spectrophotometer was designed using a light sensor and programmed to recognize changes in light intensity after passing through any solution. The devices used cost very little, approximately 3 USD, which is truly very inexpensive compared to conventional spectrophotometers costing around 10000 USD. The project aims to design and construct a spectrophotometer suitable for high school use and to validate its effectiveness through small-scale experiments determining the concentrations of Methylene Blue (MB) and Potassium Permanganate ($KMnO_4$). Preliminary results indicate the spectrophotometer's potential for simple concentration determination experiments at a reduced scale, with applications in adsorbent preparation projects. Notably, using red light (640 nm) yielded better results for MB concentration determination, while yellow light (590 nm) was more effective for $KMnO_4$. The accuracy when comparing the results with those measured by a conventional spectrophotometer was 67% and 43% for measurements with red light and yellow light, respectively. This study contributes to making spectrophotometry accessible in high school chemistry labs, even within the context of small-scale chemistry practices, fostering hands-on learning experiences.

Keywords: spectrophotometer; high school chemistry experiments; small-scale chemistry



Calibration curve for MB concentration measurement at a wavelength of 640 nm



Calibration curve for $KMnO_4$ concentration measurement at a wavelength of 590 nm

Science Projects for Students Showcase (SS-P-046)

Synthesis of zeolite from coal fly ash using the hydrothermal method and its application in ammonia treatment in water

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Many wastewater sources from industrial and domestic activities are exacerbating NH_4^+ pollution in groundwater. The research direction of treating NH_4^+ through adsorption is gaining popularity due to its high efficiency and cost-effectiveness. While the fabrication of natural adsorbent materials such as straw, rice husk ash, activated carbon, and kaolin is common, the use of coal fly ash (CFA) to synthesize zeolite in Vietnam remains limited. Specifically, the application of hydrothermally synthesized zeolite from CFA to treat NH_4^+ in water has not been widely explored. This study aims to (1) synthesize zeolite from CFA using the hydrothermal method, (2) assess its potential for treating NH_4^+ in wastewater, and (3) demonstrate its environmental benefits by reducing coal fly ash disposal. The research seeks to develop an efficient material for wastewater treatment while utilizing abundant, low-cost waste by-products, contributing to a more sustainable and eco-friendly solution for water pollution management.

Keywords: NH_4^+; coal fly ash; zeolite synthesis; wastewater treatment; hydrothermal method

Science Projects for Students Showcase (SS-P-047)

Fabrication of adsorbent material for methylene blue dye from modified water hyacinth (*Eichhornia crassipes*)

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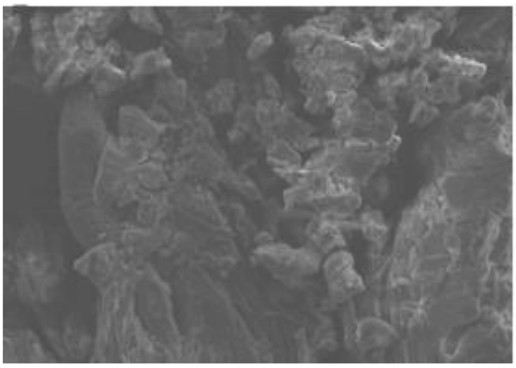
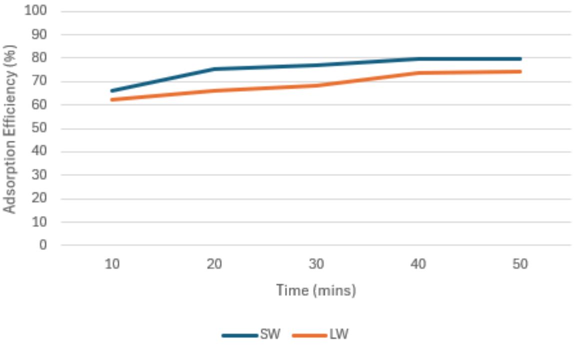
Methylene blue (MB) dye is widely used in various industries, but its stable chemical structure and resistance to degradation make it a persistent environmental pollutant. Conventional water treatment methods are often ineffective in removing MB from wastewater. This study investigates the potential of modified water hyacinth (Eichhornia crassipes), a natural and abundant resource, as an eco-friendly adsorbent for MB removal. Water hyacinth biomass, composed mainly of cellulose, hemicellulose, and lignin, was chemically modified using H_3PO_4 to enhance its adsorption capacity. The modification process yielded 28.5% of modified material from 100g of raw water hyacinth. The surface morphology of the produced material was examined using Scanning Electron Microscopy (SEM), revealing a large surface area, which contributes to enhanced adsorption capacity. The resulting adsorbent was tested for its ability to remove MB from aqueous solutions. The results showed that the modified water hyacinth stem (SW) exhibited superior adsorption compared to the modified leaves (LW). The maximum adsorption efficiency of the modified stem reached 80%, while the modified leaves achieved 74% removal. The optimal adsorption time for both materials was determined to be 40 minutes. This study demonstrates the potential of modified water hyacinth as an effective and sustainable adsorbent for the removal of MB dye from wastewater. Further research is needed to optimize the modification process and explore its application in real-world wastewater treatment scenarios.

Keywords: adsorption; methylene blue; water hyacinth; environmental treatment; wastewater purification.



STEM micrograph of the surface of the modified water hyacinth stem



The graph illustrates the MB adsorption capacity of two types of materials as a function of time.

Science Projects for Students Showcase (SS-P-048)

Collagen synthesis and remodeling 2nd degree burn wounds using bakuchiol extracted from *Psoralea corylifolia* as a plant-based agent for topical therapy

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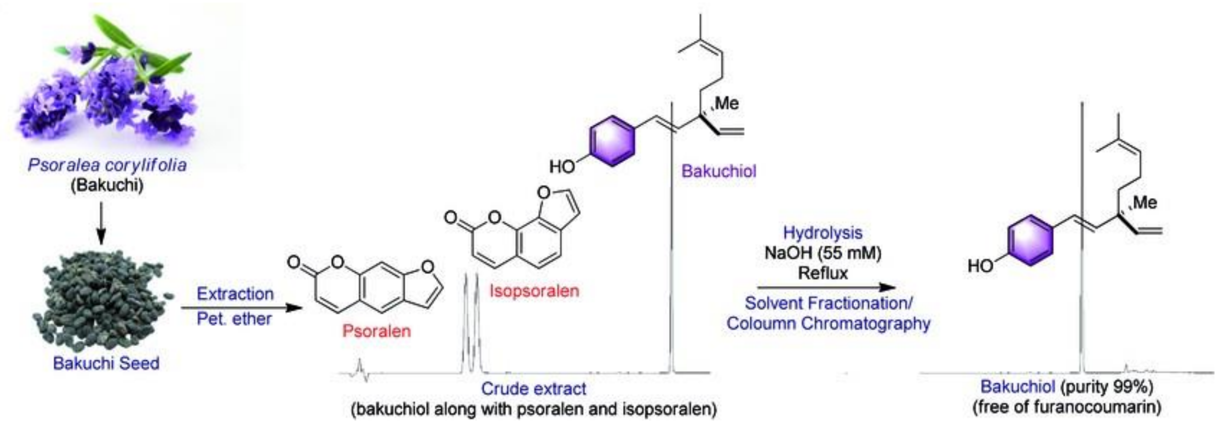
Burn injuries often lead to abnormal collagen deposition, resulting in hypertrophic scars or contractures. Traditional treatments, including silicone sheets, corticosteroids, and laser therapy, focus on scar reduction but may have limitations. Bakuchiol, a plant-derived retinol alternative, has shown anti-inflammatory, antioxidant, and pro-collagen properties, making it a potential topical agent for burn scar remodeling. Collagen remodeling is crucial in burn wound healing, as excessive or disorganized collagen deposition leads to hypertrophic scarring. This study investigates the role of bakuchiol, a bioactive compound extracted from *Psoralea corylifolia*, in enhancing collagen synthesis and remodeling in second-degree burn scars. The objectives are to: (1) analyze the effect of bakuchiol on collagen production and scar remodeling, (2) compare its effectiveness with conventional treatments such as retinoids and silicone gel, (3) assess its impact on inflammatory markers and fibroblast activity, and (4) develop a small-scale experimental approach based on green chemistry principles. The study involves in vitro and in vivo experiments, where bakuchiol's effect on fibroblast cells and burn-injured skin is analyzed. The results demonstrate that: (1) bakuchiol enhances collagen type I & III synthesis, leading to improved scar texture, (2) it reduces fibroblast overactivity and excessive scar tissue formation, (3) results in less redness and swelling, this indicate that it lowers inflammation by decreasing markers like IL-6, and Bakuchiol has been known to suppresses IL-6, a critical cytokine that drives the development of fibrosis, and (4) this small-scale experimental model provides a cost-effective, sustainable method for testing natural burn treatments. These findings suggest that bakuchiol is a promising plant-based alternative for managing burn scars, supporting innovative and eco-friendly dermatological solutions.

Keywords: collagen synthesis; burn scars; bakuchiol; green chemistry



Study on the effects of mordants on the properties of linen fabric dyed with young mango leaf extract

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Industrial synthetic dyes used in fashion and textile industries pose significant risks to both human health and the environment, particularly concerning water pollution. As the fashion industry strives to balance aesthetic demands with social and environmental responsibilities, the adoption of eco-friendly dyeing methods has emerged as a prominent trend. Among natural materials, young mango leaves have been recognized for their health benefits; however, their potential application in textile dye production remains largely unexplored. This study aims to develop a natural dye derived from young mango leaf extract and to investigate the effects of different mordants on the color properties and colorfastness of dyed linen fabric. Natural colouring agents were extracted using an aqueous extraction technique. The linen fabric then undergoes a dyeing process, using the extracts above, and then followed by mordanting using different mordant types. The dyeing performance of extracted colouring agents were assessed in terms of colour values, colour fastness properties and colour strength. The results indicate that aqueous extraction of dye from young mango leaves is a feasible method. Among the mordants examined, metal-based mordants, particularly $FeSO_4$, $CuSO_4$, and alum, exhibited the highest effectiveness in enhancing color retention and durability. Furthermore, the color fastness tests, conducted in accordance with ISO standards, provide a qualitative assessment of the fabric's resistance to washing with detergent. Future research will focus on evaluating the antibacterial properties of the dyed fabric and further analyzing the influence of mordanting temperature on the physical and chemical characteristics of the textile.

Keywords: mordants, young mango leaves, green chemistry

Science Projects for Students Showcase (SS-P-050)

The synthesis of AC/MnO_2 composite for desalination and electrodes in electrochemical supercapacitors

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Energy waste and freshwater scarcity are of global concern, with Vietnam facing significant challenges in energy inefficiency and saltwater intrusion, particularly in coastal regions like the Mekong Delta. Hence, energy storage and efficient desalination technologies are crucial aspects for contemporary research. This study investigates the synthesis of AC/MnO_2 (Activated Carbon / Manganese Dioxide) composite material for dual applications: as an electrode in electrochemical supercapacitors to address the aforementioned issues: energy storage inefficiencies and in capacitive deionization (CDI) technology for desalination. The objectives are to: (1) synthesize AC/MnO_2 composite electrodes using activated carbon from coconut shells and manganese dioxide (MnO_2), (2) evaluate their electrochemical properties, (3) assess their desalination performance via CDI, and (4) determine the feasibility of its practical implementation. The experiment is specifically conducted under 4 different conditions based on the AC/MnO_2 ratio: 100/0, 85/15, 70/30, and 50/50. Key methodologies include mechanical mixing of AC and MnO_2 with carbon black (C40) and polyvinylidene fluoride (PVDF) binder, followed by electrode fabrication and characterization using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and charge-discharge cycling (CDC). The electrochemical properties were evaluated using a three-electrode system in a 1M Na_2SO_4 electrolyte. CV was conducted within a potential window of -0.6 V to 0.6 V at various scan rates (5, 10, 25, 50, and 100 mV/s) to assess charge storage behavior, while galvanostatic charge-discharge (GCD) testing further examined at 0.1 A/g over 500 cycles. For desalination, a CDI system was employed, where asymmetric electrodes (anode: AC/MnO_2, cathode: AC) were separated by a 1 mm polyamide spacer. The system operated at 1.4 V with a 200 ppm NaCl solution (40 mL) at a flow rate of 30 mL/min, measuring salt adsorption capacity (SAC) over 60 minutes. Results demonstrate that the composite with 50% AC and 50% MnO_2 exhibits superior performance: a specific capacitance of 67 F/g at 5 mV/s, excellent stability over 500 charge-discharge cycles (260 F/g), and a high salt adsorption capacity (SAC) of 36.5 mg/g. The material's desirable properties, arising from improved charge diffusion and ion adsorption, are attributed to: (1) MnO_2's reversible Mn(IV)/Mn(III) redox transitions at surface sites enabling faradaic charge storage; (2) AC's porous structure enhancing electrical conductivity and ion adsorption capacity. The AC/MnO_2 composite functions as a dual-purpose supercapacitor electrode and desalination material, delivering high specific capacitance with robust cycling stability for energy storage and rapid salt adsorption in CDI systems. Its dual functionality as an eco-friendly, resource-abundant material provides sustainable energy storage and low-energy desalination, simultaneously tackling global energy security and freshwater scarcity challenges. The advancement aligns with the demand for integrated energy-environmental systems, offering scalable strategies for resource-constrained settings.

Keywords: energy storage; desalination; electrode composite; AC/MnO_2

Application of the RAMP system to enhance safety in chemistry laboratories: A case study of Tessaban Thakhlong 1 School

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The RAMP system (Recognize, Assess, Minimize, Prepare) is a structured approach developed to enhance safety in scientific laboratories. It emphasizes hazard identification (Recognize hazards), risk assessment (Assess risks), risk mitigation (Minimize risks), and emergency preparedness (Prepare for emergencies). Implementing the RAMP system in the chemistry laboratory at Tessaban Thakhlong 1 School promotes a culture of safety among students and teachers, reduces accidents, and improves the management of chemicals and scientific equipment. This study examines the application of the RAMP framework in an educational setting by analyzing factors influencing compliance with safety standards and developing training strategies to enhance the effective implementation of RAMP among school personnel.

Quantitative assessment revealed that accident rates decreased by 50% after the intervention, and compliance with chemical storage, waste management, and emergency preparedness standards improved from an average of 45% to 75%. The findings indicate that integrating RAMP significantly reduces laboratory safety risks and fosters a safer learning environment.

Keywords: laboratory safety; RAMP system; chemical management; school; safety culture

Science Projects for Students Showcase (SS-P-052)

Colorimetric detection of creatinine based on the peroxidase-like activity of Cu(II)-creatinine complex

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This study introduces a novel approach for creatinine analysis using a redox reaction between 3,3',5,5'-Tetramethylbenzidine (TMB) and Copper(II) nitrate hydrate. The reaction leads to a color change in the solution, which can be quantified using a UV-Visible Spectrophotometer. The absorbance increase corresponds directly to the creatinine concentration in the sample. Experimental results demonstrate that when the peroxidase-like activity of Cu^{2+}-creatinine complex interacts with TMB, the solution turns blue, with the intensity of the color becoming more pronounced as the creatinine concentration increases. A standard calibration curve was established with a linear equation of $y = 0.0091x + 0.0654$ and a high correlation coefficient ($R^2 = 0.9871$), indicating strong linearity between absorbance and creatinine concentration. The detection limit for this method was determined to be 0.0654 mg/dL. This technique offers a simple, cost-effective, and highly sensitive approach to creatinine detection, making it suitable for applications in both clinical diagnostics and biomedical research, especially in the early screening of kidney dysfunction.

Keywords: creatinine; redox reaction; UV-visible spectrophotometry

Science Projects for Students Showcase (SS-P-053)

Development of a skincare cream using madan (*Garcinia schomburgkiana* Pierre) seed extract with antioxidant and antityrosinase properties

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This study focuses on the development of a skincare cream formulated with madan (*Garcinia schomburgkiana* Pierre) seed extract, investigating its antioxidant and tyrosinase inhibitory properties. The seeds were extracted using 95% ethanol and ultrasonic waves, yielding a higher amount of crude extract compared to conventional soaking methods. Antioxidant activity, assessed via the DPPH assay, showed an IC_{50} value comparable to vitamin C, indicating strong free radical scavenging ability. Tyrosinase inhibition testing using the dopachrome method revealed IC_{50} values similar to kojic acid, suggesting skin-lightening potential. A cream containing 1% w/w madan seed extract exhibited desirable characteristics, including a light brown color, good spreadability, no phase separation, and a pH close to 6. Stability tests using heating–cooling cycles showed only minor changes in consistency. These findings highlight the potential of madan seed extract as a natural active ingredient for cosmetic formulations with antioxidant and tyrosinase-inhibiting effects.

Keywords: madan (*Garcinia schomburgkiana* Pierre) seed extract; antioxidant activity; skincare cream; tyrosinase inhibition

Science Projects for Students Showcase (SS-P-054)

Development of serum with nanoencapsulation of rambutan (*Nephelium lappaceum* L.) peel extract

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Development of serum with nanoencapsulation of rambutan (*Nephelium lappaceum* L.) peel extract. This study aimed to investigate the extraction of rambutan peel using organic solvents and evaluate its antioxidant and tyrosinase inhibitory activities. Additionally, it focused on developing a serum product containing nano-encapsulated rambutan peel extract. The extraction process employed maceration using 95% ethanol as the solvent, yielding a crude extract yield of 35.7%. Antioxidant activity tests conducted using DPPH and ABTS assays showed IC_{50} values of 0.010 ± 0.001 mg/mL and 0.008 ± 0.000 mg/mL, respectively, comparable to the standard antioxidant, vitamin C. Tyrosinase inhibitory activity revealed an IC_{50} value of 4.692 ± 2.500 mg/mL. Nanoparticles encapsulating the rambutan peel extract were developed using 1% w/w Tween80 surfactant. The resulting nanoparticles had an average size of 7.01 ± 0.17 nm, a polydispersity index (PDI) of 0.16 ± 0.03, and a zeta potential of -44.80 ± 2.39 mV, indicating good colloidal stability. Stability testing under accelerated conditions (60°C) revealed no phase separation, slight color changes, and minimal pH reduction. Antioxidant and tyrosinase inhibitory activities of the developed serum demonstrated superior efficacy compared to the base serum.

Keywords: serum; nanoencapsulation; antioxidant activity; tyrosinase inhibitory activity; rambutan (*Nephelium lappaceum* L.) peel extraction

Science Projects for Students Showcase (SS-P-055)

Development of oral care using nanoemulsion from pomegranates (*Punica granatum* L.) peel

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The objective of this research is to study the extraction of pomegranate peel using ethanol as a solvent, investigate the antioxidant of pomegranate peel extract, and develop a mouth spray product formulated with a nanoemulsion containing pomegranate peel extract. The extraction of pomegranate peel using ultrasonic waves yielded a higher crude extract percentage than the solvent-soaking method, with a crude extract yield of 18.75%. The antioxidant activity tested by DPPH and ABTS assays revealed IC_{50} values of 0.011 ± 0.001 mg/mL and 0.008 ± 0.000 mg/mL, respectively, which are comparable to ascorbic acid as the standard. In the nanoemulsion development process, Tween 80 surfactant at a concentration of 1% wt was used, resulting in nanoparticle sizes of 10.10 ± 0.54 nm, a polydispersity index (PDI) of 0.23 ± 0.06, and a zeta potential of -10.01 ± 4.95 mV, indicating good colloidal dispersion. Stability testing of the oral care product under accelerated conditions at 60°C revealed no phase separation, minimal color change, and slight pH reduction. Antioxidant activity tests of the oral care product containing nanoencapsulated pomegranate peel extract demonstrated higher antioxidant efficacy compared to the oral care product without nanoencapsulation.

Keywords: pomegranate peel extract; nanoemulsion; oral care; antioxidant activity

Science Projects for Students Showcase (SS-P-056)

Evaluation of antimicrobial properties of spices from the Zingiberaceae family

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This research aims to test the antimicrobial properties of local spice ingredients towards *Micrococcus luteus* (*M. luteus*) to study whether these local spice ingredients belonging to the Zingiberaceae family; *Zingiber officinale* (ginger), *Curcuma longa* (turmeric), and *Elettaria cardamomum* (cardamom), can inhibit the growth of *M. luteus* when extracted in different concentrations. The diffusion disc method was used to help indicate which concentration of each spice extract is most effective on inhibiting bacteria.

Ginger, turmeric and cardamom solutions were extracted and tested against *M. luteus*, using the diffusion disc method for the inhibition zone to be observed and compared for their antibacterial properties. The results show that turmeric exhibits strong consistent antimicrobial activity against *M. luteus* at all concentrations with clear and wide inhibition zones while ginger had a moderate but less consistent effect at lower concentration (1%), but showed great antimicrobial activity potential, especially at higher concentration (5%, 7%, and 10%), indicated moderate antibacterial activity that is weaker than the other two extracts.

The results highlighted that turmeric exhibited the most effective and significant antimicrobial properties against *M. luteus*, followed by ginger, showing potential at higher concentrations, and cardamom, which showed weaker activity than the other extract solutions.

Keywords: antimicrobial activity; Zingiberaceae family; *Micrococcus luteus*

Science Projects for Students Showcase (SS-P-057)

Laboratory safety practices of chemistry students at the Demonstration School of Valaya Alongkorn Rajabhat University under the Royal Patronage, Thailand

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The purpose of this study was to evaluate the safety conditions and conduct a self–assessment of the Chemistry Laboratory at the Demonstration School of Valaya Alongkorn Rajabhat University under the Royal Patronage, Phra Nakhon Si Ayutthaya Province, Thailand , using the Enhancement of Safety Practices for Research Laboratories in Thailand (ESPReL Checklist). The self-assessment, based on seven main chemical safety components, revealed that the chemistry laboratory's safety compliance scored between 40% and 60%. Specifically, chemical waste management and emergency procedures scored lower than 50%, indicating critical areas for improvement, while equipment safety management scored above 60%. Appropriate guidelines are recommended, including the implementation of training programs on hazardous waste management for teachers and students, preparation of safety manuals, and enhanced public communication. These measures are expected to elevate the laboratory's safety compliance to over 80%, reduce the risk of accidents, and foster a stronger culture of safety within the school.

Keywords: laboratory safety; safety standard; ESPReL checklist

Science Projects for Students Showcase (SS-P-058)

Water and sediment properties influencing the growth and distribution of freshwater mussels in natural water bodies in Ban Dan Lan Hoi District, Sukhothai Province

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This study aimed to analyze the properties of water and sediment and their influence on the growth and distribution of freshwater mussels. Samples were randomly collected from three natural water sources in Ban Dan Lan Hoi District, Sukhothai Province—Koetphon Reservoir, Mae Rampan Canal, and Wang Daet Canal—each at three points from October to February. Analyses followed the GLOBE Program protocol. Results indicated that Koetphon Reservoir had the highest mussel abundance, followed by Mae Rampan Canal and Wang Daet Canal. The reservoir featured brown sandy soil, no herbicide residues, clear greenish water, temperature of 25°C, transparency of 0.65–0.67 m, pH 6.5, dissolved oxygen (DO) of 8–10 mg/L, and total dissolved solids (TDS) of 18–28 ppm. The water was odorless and free of pollutants. Herbicide levels were highest in Wang Daet Canal (3 ppm), followed by Mae Rampan Canal (1 ppm), and absent in Koetphon Reservoir (0 ppm). The favorable physical and chemical characteristics of Koetphon Reservoir contribute to its suitability as a habitat for freshwater mussels.

Keywords: water properties; sediment properties; distribution; freshwater mussels

Science Projects for Students Showcase (SS-P-059)

The influence of water and sediment properties on the abundance of river snails (*Filopaludina martensi*) in natural water bodies in Si Samrong District, Sukhothai Province

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This study investigated the influence of water and sediment properties on the abundance of river snails (*Filopaludina martensi*) is a protein-rich aquatic species found in various natural water sources. This study investigates whether the characteristics of water and sediment influence the abundance of F. martensi in natural habitats. Samples were randomly collected from three points at five different locations in Si Samrong District, Sukhothai Province—Wat Ko Maidaeng Canal, Wat Nong Rang Nuea Canal, Old River Canal, Khun Kamphi Canal, and a rainwater retention pond in Wang Luek Subdistrict. Using GLOBE Program analysis methods, results revealed that the Old River Canal had the highest snail abundance, followed by Wat Ko Maidaeng Canal, Wat Nong Rang Nuea Canal, Khun Kamphi Canal, and the retention pond. The preferred habitat consisted of clayey sediment mixed with fine sand and organic matter, black in color. Water temperatures ranged from 23–25°C, transparency between 0.34–0.51 m, dissolved oxygen levels from 6–10 mg/L, pH values between 6.0–6.5, and average total dissolved solids of 15 ppm. Water color ranged from clear to black, and sediment color varied from black to brown

Keywords: water property; sediment quality; periwinkle; population density; ecological survey

Science Projects for Students Showcase (SS-P-060)

A study of natural heartwood extracts as pH indicators for use in small-scale chemistry laboratories

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This study aims to evaluate the potential of natural heartwood extracts as pH indicators for use in small-scale chemistry laboratories, aligning with the principles of green chemistry to promote safe and eco-friendly educational practices. Ethanol was used to extract color compounds from four types of heartwood: *Artocarpus heterophyllus* Lam., *Maclura cochinchinensis* (Lour.) Corner, *Artocarpus lakoocha* Roxb., and *Senna siamea* (Lam.) H.S. Irwin & Barneby. The extracts were tested across the pH range of 1–14 to observe color changes. Results showed that each extract exhibited distinct color variations at different pH levels. *Artocarpus lakoocha* Roxb. and *Senna siamea* (Lam.) H.S. Irwin & Barneby changed from light brown to dark brown at pH 9–10. *Maclura cochinchinensis* (Lour.) Corner changed from colorless to light yellow at pH 4–5 and from light yellow to dark yellow at pH 8–9. *Artocarpus heterophyllus* Lam. transitioned from opaque to light yellow at pH 4–5 and from light yellow to orange at pH 8–9. These findings indicate that heartwood extracts can serve as effective natural pH indicators for small-scale acid–base experiments, offering an environmentally friendly alternative to synthetic chemicals in educational laboratory settings.

Keywords: natural indicators; heartwood extracts; small-scale chemistry; green chemistry; acid–base reaction

Science Projects for Students Showcase (SS-P-061)

Success rate of bacteriophage therapy in treating infections caused by multi-drug resistant bacteria compared to antibiotics, and the three most commonly discussed factors influencing this rate

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The rising issue of multi-drug resistant (MDR) bacteria, such as *Acinetobacter baumannii* (AB)*,* *Klebsiella pneumonia* (KP)**,** and *Escherichia coli (E. coli)*, has posed a remarkable threat to the global health care, including the World Health Organization (WHO), requiring an alternative to conventional therapeutic approaches. Bacteriophage (phage) therapy has emerged as a potential solution in the immediate past. This research was carried out to determine its success rate and identify the three key factors influencing this rate. A literature review was executed using scientific databases such as PubMed, ScienceDirect, and Google Scholar. Studies published between 2010 and 2024 were selected based on their relevance to the application of phage therapy in combating MDR infections. Both English and Thai publications were included to provide insight into the practical implications of phage therapy for medical practitioners and pharmaceutical researchers. The findings indicate that the success rate is 90%. Furthermore, the data imply that the three key factors influencing the success rate are (1) phage-host specificity (2) combination with antibiotics, and (3) development of phage resistance. Nevertheless, the review confirmed that phage therapy has its limitations, emphasizing the need for further research to enhance its integration into modern healthcare systems as an alternative to antibiotics.

Keywords: multi-drug resistant bacteria; *Acinetobacter baumannii*; *Klebsiella pneumonia*; *Escherichia coli*; bacteriophage therapy

Science Projects for Students Showcase (SS-P-062)

Development of chitosan and *N*,*O*-carboxymethyl chitosan coating with stearic acid to increase amide bond formation and transparency

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This research aim to develop a coating materials from Chitosan and *N*,*O*-carboxymethyl chitosan (CMC) with stearic acid for transparent films. The experiment consisted of two parts 1) Formation of Amind bonds in Chitosan and CMC Coatings. The films were prepared by dissolving stearic acid and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC) in ethanol, then mixing with Chitosan in acetic acid and CMC films were prepared similarly using distilled water. FTIR analysis showed a clear peak at 1632 cm^{-1}, confirming amide bond formation. Chitosan films exhibited stronger amide peaks, suggesting greater crosslinking and structural integrity. 2) Effect of Stearic Acid Concentration Chitosan films were prepared with stearic acid concentrations of 0.2, 0.4, and 0.8 g. The film containing 0.2 g stearic acid exhibited the highest light transmittance at 81.30 ± 0.41% and the greatest amide bond formation. The other films showed lower transmittance due to their viscous nature, which hindered proper dispersion during formation. Conclusion: The chitosan film containing 0.2 g of stearic acid exhibited the highest amide bond formation and the greatest transparency. These results are attributed to the low concentration of stearic acid. Therefore, this formulation shows high potential for application as a self-cleaning surface coating.

Keywords: N,O-carboxymethyl chitosan; chitosan; stearic acid; films

Science Projects for Students Showcase (SS-P-063)

Sugarcane derived nitrogen-doped carbon dots based fluorescence detection of formaldehyde with dual sensing ranges

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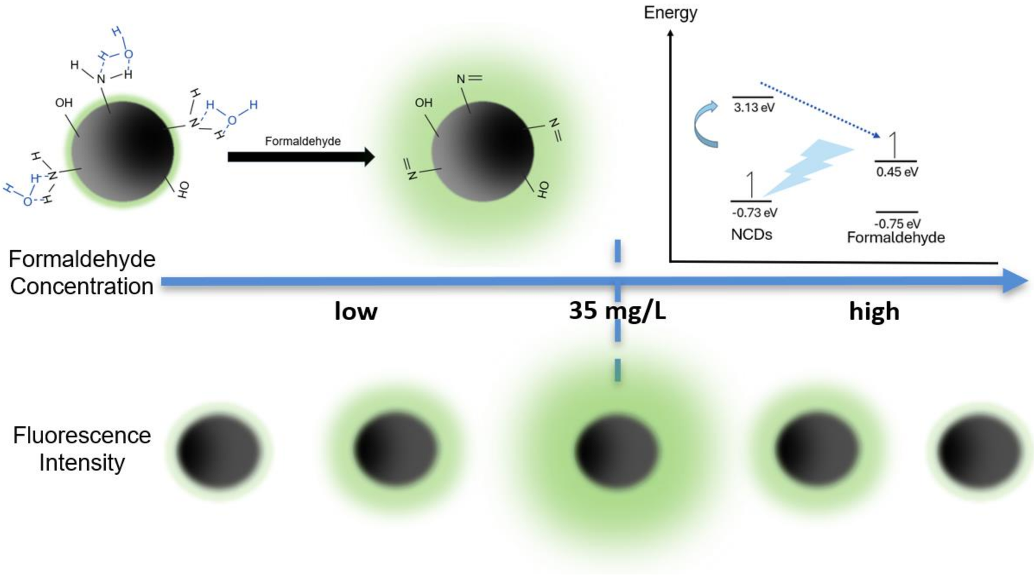
Formaldehyde, a class I carcinogen, is widely used for food preservation, tableware, and fumigation. Carbon dots (CDs), the carbon nanoparticle, are one of promising methods for detection of formaldehyde via fluorescence signal due to their unique photoluminescence properties, high selectivity and sensitivity. However, there were two contradicted reports, the increasing and decreasing fluorescence intensity towards formaldehyde. This work aims to study the mechanisms behind those two different responses and fabricate a sugarcane derived carbon dots-based fluorescence sensor with two different modes of responses. The extracted lignin from sugarcane bagasse and m-phenylenediamine (MPDA) was used to synthesize nitrogen doped carbon dots (NCDs) via hydrothermal method. It was found that the fluorescence intensity increased upon the increasing of formaldehyde concentrations before starting to fall after exceeded 35 mg/L. The calculated energy level of NCDs and FT-IR spectrum led to the proposed mechanism is, at lower concentration of formaldehyde, NCDs form Schiff's base product, disrupting the hydrogen bonds with solvent, resulting in the rising of fluorescence intensity which is first-ordered with respect to formaldehyde. At higher concentration, the photo-induced electron transfer (PET) from NCDs to formaldehyde, which is thermodynamically favorable and second-ordered with respect to formaldehyde, becomes dominant, leading to the drop of intensity.

Keywords: formaldehyde; fluorescence detection; nitrogen-doped carbon dots; photo-induced electron transfer; sugarcane bagasse



Science Projects for Students Showcase (SS-P-064)

The comparison of the effectiveness in inhibiting the germination of cress seeds by the extracts of kale stems, water spinach stems, and corn husks

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Kale stems, water spinach stems, and corn husks are parts that are not commonly consumed. If these are used to extract secondary metabolites to inhibit the germination of *Cress* seeds, it would be an effective way to reduce food waste. This study aims to 1) extract the secondary metabolites from all of them using distilled water, and 2) compare the effectiveness of these extracts in inhibiting the germination of *Cress* seeds. The method involved applying the extracts of plants with different concentrations to *Cress* seeds, watering them continuously for 20 days, with a control group watered with distilled water. There were three experimental groups, each of which had three concentrations: 50, 75, and 100 grams of dry weight per liter. Each concentration was repeated three times. Changes were observed by measuring the root and stem lengths. The results showed that all the extracts did not inhibit germination. The seeds treated with the plant extracts are still germinated with roots and stems growing. The root lengths were not significantly different from the control group. However, the average stem lengths were shorter than the control group, indicating that the extracts from all three plants could inhibit the growth of the *Cress* stems.

Keywords: secondary metabolites; food waste; herbicide

Investigating the effectiveness of different concentrations of sodium fluoride in preventing cavities

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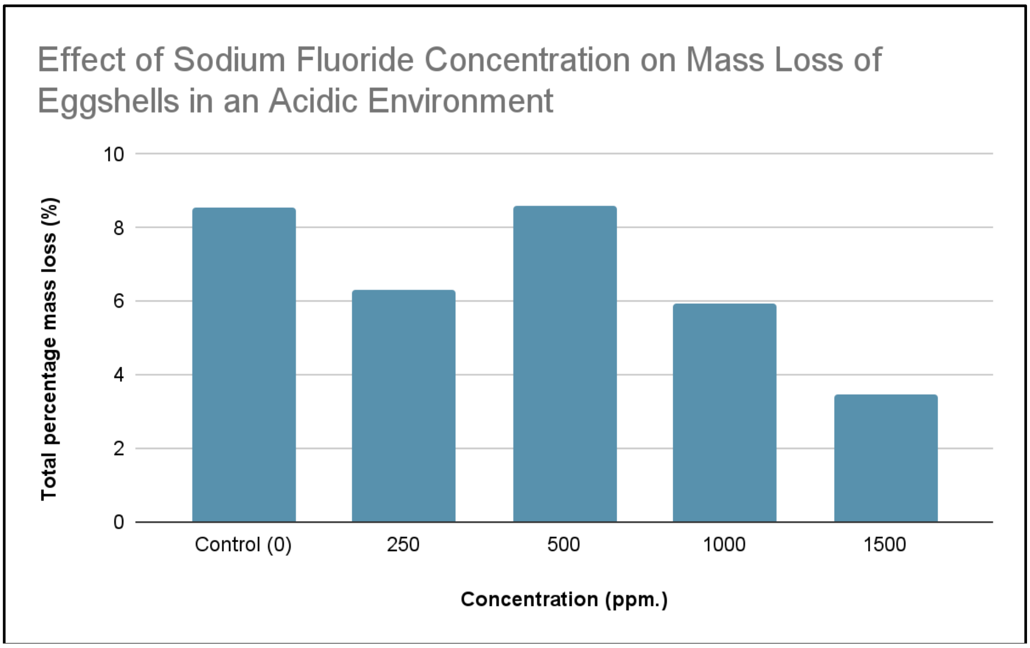
This study examines the role of sodium fluoride in protecting tooth enamel from demineralization, using eggshells as a model due to their similar calcium content and structure. Eggshells of uniform initial mass (~5g each) were used. Samples were soaked in sodium fluoride solutions of varying concentrations (0, 250, 500, 1000, and 1500 ppm) for 20 hours, then exposed to vinegar (5% acetic acid; pH 2.5–3.0) for another 30 minutes to simulate acidic conditions. Only one concentration of vinegar was used.

Results showed a negative correlation between fluoride concentration and mass loss, with the control group having the highest mass loss (8.57%), while 1000 and 1500 ppm resulted in significantly lower losses (5.96% and 3.46%). An anomaly at 500 ppm showed an unexpected increase in mass loss, indicating potential experimental errors. The study supports fluoride's role in strengthening enamel and enhancing remineralization. However, excessive fluoride exposure carries a risk of dental fluorosis, which often occurs when fluoride concentrations exceed 1.5 ppm in drinking water or from prolonged use of high-fluoride toothpaste. These findings highlight the importance of balanced fluoride use in dental care and public health to maximize benefits while minimizing risks.

Keywords: sodium fluoride; enamel; demineralization; dental fluorosis



Enhancing biomass and protein contents in *Schizophyllum commune* mycelium cultivated in liquid culture and its application as an alternative protein source

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Mushroom farming is a process that generates significant waste, including leftover substrate, spent mushroom compost, and maintenance-related waste, contributing to negative environmental impact. Mycelium production offers an alternative to traditional mushroom farming, providing a more sustainable approach to mushroom agriculture. This study explored cultivation conditions to enhance the production of mycelium with higher biomass and protein content and investigated its potential use in a food product. Mycelium of *Schizophyllum commune* was grown on agar with different carbon sources (sucrose or glucose), varying concentrations of nitrogen source (from *Morus alba* leaf crude extract), and calcium chloride. Then, the condition with high biomass yield and protein content was applied to liquid culture for further investigation. The result showed that the media which provided highest biomass yield and protein content was sucrose, 4 mg/g *Morus alba* leaf crude extract and 3 g/L $CaCl_2$. The cultivation condition was used to harvest mycelium for incorporating into drinking jelly containing different gelling agent (carrageenan, konjac powder and locust bean gum) and varying sweetener (honey and fructooligosaccharide). Sensory evaluation revealed that the drinking jelly with mycelium had high acceptance scores.

Keywords: alternative protein; mycelium cultivation; liquid cultivation; *Schizophyllum commune*

Science Projects for Students Showcase (SS-P-067)

Comparison of lead(II) ion adsorption efficiency between cellulose phosphate and cellulose phosphate-silica

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This study aims to investigate and compare lead adsorption efficiency in aqueous solution of modified sugarcane bagasse-derived cellulose fibers which are cellulose phosphate and cellulose phosphate combined with silica. Adsorption times are varied at 30, 45 and 60 minutes and the initial concentration of lead(II) ions was prepared at 40 ppm. Quantitative analysis of the remaining of lead(II) ions in aqueous solution was operated by UV-Vis spectrophotometry after complexation with 0.01% w/v Eriochrome Black T. Adsorption efficiency was then calculated based on the difference between initial and final concentration of lead(II) ions. Physical characteristics of the adsorbents were analyzed using Scanning Electron Microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FTIR) was employed to determine their chemical compositions. Linear equation obtained from the standard curve of lead solution was $y = 0.0028x + 0.2151$ ($R^2 = 0.9909$). Experimental results demonstrated that adsorption efficiency of sugarcane bagasse-derived cellulose fibers, cellulose phosphate, and cellulose phosphate combined with silica at 30, 45 and 60 minutes adsorption time were 20.63±0.73, 32.53±4.39, 40.86±2.95, 30.74±4.39, 36.10±4.45, 53.96±2.95, 41.46±2.56, 53.96±2.95 and 81.34±0.73, respectively. The results indicated that adsorption efficiency increased with longer adsorption times. Cellulose phosphate and cellulose phosphate combined with silica possessed higher adsorption efficiency when compared with that of sugarcane bagasse-derived cellulose fibers, and cellulose phosphate combined with silica exhibited the highest adsorption efficiency. The findings suggest that modifying sugarcane bagasse-derived cellulose fibers through phosphorylation and combining with silica can significantly enhance lead adsorption efficiency. This study proposes alternative material and fundamental data for future development of natural cellulose-based adsorbents for heavy metal removal in aqueous solution.

Keywords: adsorption efficiency of lead(II) ions; sugarcane bagasse-derived cellulose fibers; cellulose phosphate; cellulose phosphate combined with silica; UV-vis spectrophotometry

Science Projects for Students Showcase (SS-P-068)

Extraction of protein micelles from soy protein powder to stabilize chocolate

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This study aimed to evaluate the heat resistance of chocolate by incorporating micellar protein at concentrations of 4%, 6%, 8%, 10%, and 12%. For each formulation, chocolate samples with volumes of 3, 4, 5, 6, and 7 mL were prepared and subjected to heat resistance testing at temperatures of 25°C, 35°C, 45°C, and 55°C. Each experimental condition was performed 10 times to ensure the reliability and credibility of the reported average heat resistance times. In the first experimental set, chocolate containing 4% micellar protein showed that a 6 mL sample exhibited average heat resistance times of 12.45, 8.39, 4.02, and 4.05 minutes, respectively. In the second set, with 6% micellar protein, a 7 mL sample demonstrated average heat resistance times of 13.02, 11.02, 8.00, and 6.85 minutes. The third set, incorporating 8% micellar protein, indicated that a 5 mL sample had average heat resistance times of 15.05, 14.00, 11.54, and 8.70 minutes. The fourth set, containing 10% micellar protein, revealed that a 5 mL sample exhibited the highest heat resistance, with average times of 27.03, 22.53, 17.28, and 13.00 minutes. Finally, in the fifth set, using 12% micellar protein, a 3 mL sample demonstrated average heat resistance times of 17.06, 13.33, 12.04, and 9.65 minutes. The experimental results indicate that the chocolate formulation containing 10% micellar protein at a sample volume of 5 mL exhibited the highest heat resistance across all tested temperatures (25, 35, 45, and 55°C). These findings suggest that micellar protein plays a crucial role in enhancing the thermal stability of chocolate, making it a potential functional ingredient for improving chocolate resilience under elevated temperatures.

Keywords: chocolate; micelle; protein micelle; soy protein

Science Projects for Students Showcase (SS-P-069)

Lac paper sensors for detecting lead in solution

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This project aims to study the appropriate conditions for creating a paper sensor to measure lead concentration in a solution by observing the color resulting from the complex reaction of lead solution with lac extract. This project was studied the reaction area conditions, paper type, lac extract volume, pH value, reaction time, and lead specificity. In each step, the condition that gives the highest color change (ΔE) will be selected for further study in the next step. From the results, it was found that the condition that gives the highest color change (ΔE) is chromatography paper with a reaction area of 0.50 * 0.50 square centimeters, together with a lac extract volume of 6 μL at pH 7.45, after reaction time for 2 minutes. When tested with other heavy metals, it was found that the paper sensor is not specific to other heavy metals, but will give different colors for each type. Therefore, this point can be further developed to identify and create specificity for heavy metals.

Keywords: colorimetric sensor; heavy metal; ΔE; natural dye

Science Projects for Students Showcase (SS-P-070)

Evaluation of the efficiency of hard capsules from hydroxypropyl methylcellulose and pomelo peel pectin

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This study aimed to evaluate the effectiveness of hydroxypropyl methylcellulose (HPMC) and pectin from pomelo peel as alternative materials to gelatin for hard capsule production. Capsule films were prepared with HPMC and pectin at ratios of 50:50, 60:40, 70:30, 80:20, 90:10, and 100:0. The disintegration times were measured in pH 7 and pH 2 solutions. Capsules with a 50:50 ratio began disintegrating within 48 minutes due to the lower HPMC content, which lower acid resistance. In contrast, capsules with higher HPMC ratios (60:40 to 100:0) showed longer disintegration times, as increased HPMC content enhanced capsule strength and delayed breakdown. The results demonstrate that HPMC and pomelo peel pectin can serve as alternative materials for capsule production. Pectin improves mechanical strength, while HPMC enhances flexibility. This combination supports the development of capsules for consumers who avoid gelatin and promotes the sustainable use of natural materials in pharmaceutical and food industries.

Keywords: hydroxypropyl methylcellulose; pectin; pomelo peel; hard capsules; disintegration

Science Projects for Students Showcase (SS-P-071)

Research and comparison of the amount of protein in *Wolffia globosa* fed with different fermentations

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The objective of this project is to develop and compare food formulas for cultivating Wolffia globosa (commonly known as watermeal or duckweed) with high protein content. This aims to address the issues of high animal feed prices and the shortage of quality natural protein sources. It will enable both farmers and consumers to have greater access to sustainable and environmentally friendly alternative protein sources in the future. Additionally, using Wolffia in animal feed formulas or for direct consumption may also help alleviate the impact of rising meat prices in the long run. Cultivation environments Wolffia We have control factors is set the ph at 5-6 in a sunny area. The water temperature is about 20-26 °C. Based on the measurement of Wolffia growth from dry weight and wet weight, it was found that Wolffia cultivated with photosynthetic bacteria had the highest growth, followed by Wolffia cultivated with a mixture of bio-fermented plant water and photosynthetic Bacteria (ratio 1:2). The Wolffia with the lowest growth was cultivated with a mixture of bio-fermented animal manure water and photosynthetic Bacteria (ratio 1:2). From the study of protein content in Wolffia powder, using the standard graph, OD value table, and the equation $y=0.8762x+0.0677$ to calculate the protein content, it was found that Wolffia powder cultivated with a mixture of bio-fermented plant water and photosynthetic bacteria (ratio 1:2) had the highest protein content. This was followed by Wolffia powder cultivated with a mixture of bio-fermented animal manure water and photosynthetic bacteria (ratio 1:2). The Wolffia powder with the lowest protein content was cultivated solely with photosynthetic bacteria.

Keywords: Wolffia; growth; high protein

Science Projects for Students Showcase (SS-P-072)

Examination of the factors that influence the morphology and size of nanofibers produced from silk protein extract in conjunction with PVA

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The study aimed to investigate key parameters influencing the morphology and diameter of the resulting nanofibers. The electrospinning process was optimized by varying the ratio of silk protein extract to 10% (w/v) PVA, the applied voltage (15 kV and 18 kV), the solution flow rate (0.8, 0.9, and 1 mL/h), and the needle gauge size (18, 20, and 21). The physical characteristics of the nanofibers were subsequently analyzed using scanning electron microscopy (SEM). The experiment revealed that key factors influencing the formation of nanofibers via electrospinning include applied voltage, flow rate, needle size, and the ratio of silk protein extract to PVA. Analysis of applied voltage (15 and 18 kV) using an independent t-test showed no statistically significant difference ($p = 0.709$); however, 15 kV tended to produce finer and more aligned fibers. For flow rate (0.8, 0.9, 1.0 mL/h), needle size (18, 20, 21 gauge), and silk protein:PVA ratios (0:100, 10:90, 20:80), one-way ANOVA was used. The p-values for flow rate and needle size were 0.129, indicating no significant differences, though 0.8 mL/h and needle size 18 showed trends toward producing the smallest and most uniform fibers. In contrast, the silk protein:PVA ratio of 20:80 resulted in the smallest average fiber diameter (270.28 ± 51.67 nm) with a statistically significant difference ($p < 0.05$), indicating that the composition of the spinning solution plays a crucial role in determining fiber quality.

Keywords: nanofibers; electrospinning; scanning electron microscopy (SEM)

Science Projects for Students Showcase (SS-P-073)

Development of an indicator film from butterfly pea (*Clitoria ternatea*) extract for monitoring the sourness level of the pork products (Naem Moo)

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This project develops an innovative indicator film derived from butterfly pea flower (*Clitoria ternatea*) extract, rich in anthocyanins, which serve as natural pH indicators to assess the acidity levels of fermented pork (Naem Moo) during the fermentation process. The film is meticulously crafted by blending anthocyanin extract with agar, forming a thin, transparent, and flexible material that exhibits distinct color shifts in response to pH variations. To evaluate its performance, the film was tested with buffer solutions across a pH range from 1 to 9. It exhibited distinct color changes, showing red at pH values of 1 and 2, purple at pH values from 4 to 6, and blue to green at higher pH levels. Since Naem Moo typically has a pH around 4, the film turned purple when applied to actual samples, matching the buffer color at that level. This technique empowers producers and consumers to easily assess freshness and ensure quality during fermentation, improving food safety and confidence.

Keywords: indicator film; anthocyanin; pork products (Naem Moo); pH measurement

Science Projects for Students Showcase (SS-P-074)

Investigation of the physical and chemical properties of bioplastics derived from durian peel cellulose

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Carboxymethyl cellulose (CMC) is widely used in bioplastic production and is typically derived from wood-based cellulose, which may contribute to deforestation. This study aimed to synthesize CMC from durian peel, an agricultural waste, and compare the properties of bioplastics made from durian peel CMC and commercial CMC. Cellulose was extracted from durian peel and converted into CMC via carboxymethylation, then characterized using FT-IR spectroscopy. Bioplastic films were prepared by blending 1.0, 1.5, and 2.0 g of CMC with chitosan and glycerol. The films were evaluated for tensile strength, water solubility, and biodegradability. The film containing 1.5 g of durian peel CMC showed the highest tensile strength (10.59 N), not significantly different ($P > 0.05$) from that of commercial CMC (10.92 N). The lowest water solubility was 7.4% for 1.5 g durian CMC, also not significantly different ($P > 0.05$) from 5.1% for 2.0 g commercial CMC. Both types of bioplastics began degrading on day 2 and were fully degraded by day 6. Films from durian peel CMC appeared translucent, slightly yellow, and rough, whereas commercial CMC films were clear and smooth. These findings suggest that durian peel CMC is a promising, eco-friendly alternative for sustainable bioplastic production.

Keywords: carboxymethyl cellulose (CMC); bioplastic; durian peel

Science Projects for Students Showcase (SS-P-075)

Development of a simple microfluidic paper sensor with image processing analysis for early detection of chronic kidney disease

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Chronic kidney disease (CKD) is an increasingly significant public health concern. Early detection can be achieved by screening for microalbumin levels in urine. However, conventional methods are often costly and time-consuming. To address this limitation, a microfluidic paper sensor was designed and fabricated using a simple microfluidic technique. The sensor operates based on a colorimetric reaction between microalbumin and Tetrabromophenolphthalein ethyl ester (TBPE), an organic compound. This reaction, which occurs between an organic molecule and a protein, induces a chemical structural change that leads to a visible color shift in the organic reagent. An image processing program was employed to analyze the average color intensity from sensor images, enabling the preliminary classification of CKD stages. Two paper designs were tested type 1 and type 2. When evaluated using synthetic urine containing Bovine Serum Albumin (BSA) at concentrations of 10, 20, 30, 40, and 50 mg per 100 mL, the paper type 2 demonstrated superior performance. This was attributed to its ability to distinctly separate reaction zones and more effectively control fluid flow. The image-processing algorithm successfully classified CKD stages with 95% accuracy and an average processing time of 0.0083 minutes. These findings suggest that the proposed microfluidic paper sensor is a promising, efficient, and low-cost tool for early-stage CKD screening.

Keywords: microalbuminuria; microfluidic paper; image processing

The study of lead adsorption ability of pectin hydrogel from sugar palm fibers combined with carbon quantum dot particles from mangosteen peel

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Heavy metal contamination in water poses serious environmental and health risks as toxic metals accumulate in aquatic life and enter the human food chain. Among various treatment methods, adsorption is cost-effective and simple. This project explores the use of pectin hydrogel combined with carbon quantum dots (CQDs) to enhance lead (II) ions (Pb^{2+}) removal from water. Mangosteen peels, a form of agricultural waste, are used to synthesize CQDs rich in functional groups of hydroxyl, carbonyl, and amine, which bond effectively with heavy metal ions. Sugar palm fibers, also discarded agricultural material, are a source of pectin for hydrogel formation. The pectin hydrogel contains carboxylic groups that also facilitate heavy metal adsorption. Experimental results indicate that pectin hydrogel can adsorb approximately 6.53 ± 0.07 mg/g of lead within 100 minutes. In comparison, a composite of pectin hydrogel and carbon quantum dots (CQDs) with 1:4 ratio achieves the highest adsorption capacity, of 11.38 ± 0.31 mg/g with the same adsorption time. The findings demonstrate that the incorporation of CQDs enhances the lead adsorption efficiency of pectin hydrogel ($p < 0.05$). However, increasing the amount of carbon quantum dots beyond this ratio does not enhance adsorption efficiency.

Keywords: carbon quantum dots; pectin hydrogel; heavy metal; lead adsorption

Science Projects for Students Showcase (SS-P-077)

Study on factors affecting the activity of lipase enzyme to accelerate the biodegradation of PBS bioplastic

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The plastic waste problem is a significant environmental issue, as conventional plastics take hundreds of years to degrade. This leads to waste accumulation and pollution in ecosystems. However, biodegradable plastics, such as Polybutylene Succinate (PBS), can be decomposed by microorganisms in nature. Despite this, the degradation process remains slow. This project aims to investigate the factors influencing the activity of lipase, an enzyme capable of accelerating PBS degradation, to enhance the efficiency of biodegradable plastic decomposition. The experiment was divided into three parts. In the experiment, the plastics were immersed in solutions under various conditions and the enzyme performance was analyzed by weighing the mass of the remaining plastics, washing with distilled water, drying thoroughly and weighing them on a scale. SEM was also used to compare whether the deterioration of the surface corresponded to the experimental results by weighing the mass. First, the effect of enzyme concentration was examined, revealing that an 8% v/v concentration was optimal for accelerating PBS degradation. Second, the effects of pH and metal ions were studied, showing that a pH of 7 and the addition of Mg^{2+} resulted in the highest degradation rate. Finally, a comparison between natural degradation and enzymatic degradation demonstrated that the use of lipase, in combination with optimal factors, significantly accelerated PBS decomposition compared to natural processes. The findings indicate that utilizing lipase with appropriate conditions can enhance the degradation rate of PBS, offering a more efficient approach to biodegradable plastic decomposition.

Keywords: lipase enzyme; polybutylene succinate (PBS); biodegradation

Science Projects for Students Showcase (SS-P-078)

Development of carboxymethyl cellulose-activated carbon composite hydrogel with citric acid crosslinking for cationic dye adsorption in sustainable wastewater treatment

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At present, wastewater from the textile industry and local dyeing communities—such as the Ban Nong Sang handwoven group in Nakhon Phanom Province—raises environmental concerns due to the discharge of untreated cationic dye-contaminated water. Effective, reusable, and biodegradable wastewater treatment materials are therefore essential. This project aims to compare the adsorption efficiency of different composite hydrogels for cationic dyes, evaluate their reusability, and examine the quality of dye released from the hydrogels for potential reuse in fabric dyeing. The study found that hydrogel type 10, composed of 4 g carboxymethyl cellulose, 1.6 g activated carbon, and 2% citric acid, achieved the highest methylene blue dye adsorption efficiency at 99.3%. The hydrogel's network structure offered a good balance between mechanical strength and swelling capacity. However, increasing citric acid concentration beyond 2% reduced adsorption efficiency due to excessive crosslinking.

Regarding reusability, hydrogel types 6, 9, and 3 showed the least performance decline—1.3%, 1.4%, and 1.8% respectively—and remained effective for up to four cycles. Hydrogel type 9 offered an optimal balance, with 98.9% adsorption efficiency and minimal reduction after repeated use. These findings indicate the developed composite hydrogel holds strong potential as a sustainable and eco-friendly wastewater treatment material that also reduces the need for new dyes and lowers treatment costs.

Keywords: composite hydrogel; carboxymethyl cellulose; activated carbon; adsorption; cationic dye; wastewater treatment; sustainability

Science Projects for Students Showcase (SS-P-079)

Herbal soap for antibacterial protection against skin diseases from cardamom, cat's whiskers, and stevia

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This study shows the importance of keeping the body free from Staphylococcus aureus, which is the cause of dermatitis, abscesses, and blisters. The infection can spread through contact. This study shows the importance of keeping the body free from infectious fungi and contaminated objects. The objective of the study is to develop herbal soap with antibacterial properties. The experiment used 3 herbs: cardamom, Orthosiphon stamineus, and sweet grass. Cardamom has the ability to inhibit the growth of some bacteria, Orthosiphon stamineus helps prevent infection and relieve joint pain, and stevia has substances that inhibit the spread of bacteria that cause skin diseases. All 3 herbs have the ability to inhibit the growth of some microorganisms. The experimental method uses the culture method. Plates 1-3 are dropped with stevia, cardamom, and sweet grass separately in each plate. Plate 4 includes all 3 herbs, and plate 5 does not add any herbs. In the Petri dish, bacteria from the skin area were left for 2 weeks. It was found that in Plate 1, cardamom and Plate 4, mixed herbs, the bacteria in the Petri dish did not grow. From the conclusion, the three herbs helped reduce bacteria in the body. However, Plates 2 and 3 had bacteria remaining, but when compared to Plate 5, there were fewer bacteria. From the study, which tested the bacteria in the Petri dish, which is the cause of skin diseases, it was found that all three herbs were effective in preventing skin diseases. This shows that they can be developed into cleaning products with antimicrobial properties. This experiment should be further studied to be an alternative for further development.

Keyword: herbal soap ; cardamom ; orthosiphon stamineus ; stevia ; antibacerial ; skin diseases

Science Projects for Students Showcase (SS-P-080)

Green synthesis of silver nanoparticles using five varieties of *Vitis vinifera* (grape) leaf extract and determining their antioxidant property, antibacterial activity, photocatalytic property, cytotoxicity and detecting melamine adulteration

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This study was conducted to synthesize silver nanoparticles (AgNPs) using five varieties of *Vitis vinifera* extract such as, Cardinal, French-M.I, Muscat-M.I, Isabella and Israel-blue. The phytochemicals required for capping, nucleation, bio-reduction and stabilizing of AgNPs was confirmed through qualitative analysis using grape water extract. Biosynthesis of AgNPs was initially observed by color change and further confirmed by UV-Visible spectroscopy with a band between 440nm-480nm in all five varieties. Scanning electron microscope images confirmed the shape of Israel-AgNPs as spherical and size in range of 50nm-60nm. Further antioxidant assays such as TFC, TPC and TAC were performed. AgNPs had higher antioxidants than water extracts. Based on antioxidant results, Israel-AgNP was utilized for further investigation. Melamine was detected in raw milk using Israel-AgNP. Degradation of methylene blue was monitored under sunlight and with $NaBH_4$ in the presence of Israel-AgNP and shows fully degradation of the dye. Zone of inhibition studies revealed AgNPs has noteworthy antibacterial potential against *Escherichia coli* and *Staphylococcus aureus*. One-way ANOVA indicated a statistically significant difference between grape water extracts and AgNPs as Pvalue<0.05 and Fvalue>Fcrit for TFC, TPC, TAC and antibacterial activity. Cytotoxicity test was performed against brine shrimps and presented 100% viability rate after 24hours. Therefore, grape AgNPs can be used in bioremediation and drug development.

Keywords: silver nanoparticle; photocatalysis; melamine adulteration; antibacterial

Science Projects for Students Showcase (SS-P-081)

Effects of orchid (*Dendrobium sp.*), marigold (*Tagetes erecta L.*), and lotus (*Nelumbo nucifera Gaertn.*) crude extracts on growth of popping pod (*Ruellia tuberosa Linn.*)

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According to Thailand's religious culture, orchid, marigold, and lotus are some of the flowers that are mainly used and become waste. Along with weed problems in agriculture, this research aims to test orchid, marigold, and lotus extracts that can inhibit minnieroots growth, a common weed in Thailand. By using dried-blended flowers to produce crude extracts, allelochemicals in the flowers are released and can affect the growth of minnieroots, also reducing flower waste all at once. Each flower extract was used at three concentration levels: 50, 75, and 100 grams of dry weight per liter (g(DW)/L) with two solvents: distilled water and methanol at 95% v/v. Each solution was given to the minnieroots, then watered for 30 days. The growth of minnieroots in the control group, which only receives water, was compared to the group that receives flower extracts. Results show that the solution extracted with methanol, which has shorter average root and stem length, can inhibit the growth of minnieroots over distilled water. From the results, at 50 g(DW)/L solution extracted with methanol from all three types of flower extract has the most ability to inhibit the stem and root growth of minnieroots (non-germination), compared to all mentioned groups.

Keywords: weed control; flower extracts; allelochemicals; flower waste management

Science Projects for Students Showcase (SS-P-082)

In silico investigation of a library of acetaminophen-based ester derivatives for antibacterial potential through molecular docking and drug-likeness studies

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Drug-resistant bacteria are straining healthcare systems, demanding urgent new antibacterials. Acetaminophen derivatives are promising candidates due to their favorable pharmacokinetics and modifiable functional groups. This study investigates 40 acetaminophen-based ester derivatives, incorporating *ortho*-, *meta*-, and *para*- substitutions to examine electronic and steric effects. In silico pharmacokinetic screening, using the BOILED-Egg model and Lipinski's Rule of Five, identified four promising candidates (M13, M22, M25 and M28). Moreover, molecular docking against bacterial targets including Penicillin-Binding Protein 2a (1MWT), Staphylocoagulase (1NU7), FimH adhesin (4XO8), and DNA gyrase from *Staphylococcus aureus* (3G7B) and *Escherichia coli* (1KZN) revealed binding affinities ranging from -5.8 to -7.6 kcal/mol. Notably, M25_*meta* and M28_*meta* (bearing carboxylate and carboxamide side chains) exhibited the lowest average binding affinities across multiple bacterial targets, with values of –6.94 and –6.88 kcal/mol, respectively, while M25_*para* and M28_*para* showed higher averages of –6.70 and –6.84 kcal/mol. These results suggest that *meta*-substituted derivatives may exhibit stronger and more stable interactions that favor competitive binding against the enzymes' native substances by lowering the system's binding energy. Therefore, these findings provide insights into the structure-activity relationships of acetaminophen-based esters as antibacterial agents and highlight *meta*-substituted derivatives as promising candidates for further optimization.

Keywords: acetaminophen derivatives; in silico screening; molecular docking; antibacterial agents; *meta*-substituted

Science Projects for Students Showcase (SS-P-083)

A paper-based perfluoro octane sulfonic acid (PFOS) detection using amine-functionalized carbon dots

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Perfluoro octane sulfonic acid (PFOS) is widely used across various industries but persists in the environment and human bodies due to its difficulty in decomposition. Current PFOS detection techniques face challenges, such as high costs, complex processes, and long analysis times. Herein, an easy and rapid PFOS detection method using carbon dots (CDs) functionalized amine with the addition of Fe^{3+} was studied. Initially, Fe^{3+} quenched the fluorescence (FL) intensity of CDs. However, in the presence of PFOS, Fe^{3+} interacted with PFOS, restoring FL intensity. CDs functionalized with three different amine compounds were synthesized and tested. Among them, 1% v/v CDs-urea, exhibiting the highest significant fluorescence light (FL) intensity change by naked eyes under the UV light, was coated onto paper-based devices. After adding a PFOS-containing sample pre-mixed with Fe^{3+} solution onto the device, the FL quenching distance was measured within 15 minutes. Higher PFOS concentrations resulted in shorter quenching distances. The device demonstrated the limit of detection of 0.578 µg/L, the sensitivity of 0.8985 cm/log(µg/L), and the linearity of 62.5 - 2000 µg/L. However, interference from HCO_3^-, SO_4^{2-}, and Cl^- was observed. This paper-based device presents a promising, rapid, and user-friendly tool for effective environmental PFOS monitoring.

Keywords: perfluoro octane sulfonic acid (PFOS); carbon dots (CDs); urea, cysteine; cysteamine

Science Projects for Students Showcase (SS-P-084)

Study on the extraction of compounds from the leaves and shoots of Saudi Bael (*Schinus terebinthifolia* Raddi) using ultrasonic extraction and evaluation of antioxidant activity

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This study focuses on the extraction of compounds from the leaves and shoots of Saudi Bael (*Schinus terebinthifolia* Raddi) using ultrasonic extraction and the evaluation of its antioxidant activity. The extraction was carried out using 95% ethanol, and the ultrasonic extraction method was compared with traditional solvent soaking extraction. The results showed that ultrasonic extraction yielded higher amounts of crude extract, with the highest yield from the shoots of Saudi Bael (14.95%) and from the leaves (9.70%). Additionally, the antioxidant activity was assessed using the DPPH Radical Scavenging method. The results revealed that the extract from the shoots exhibited significant antioxidant (IC_{50} = 0.0501 mg/ml). This indicates the potential of Saudi Bael shoot extract as a source of antioxidants, suitable for the development of antioxidant-rich products.

Keywords: Saudi Bael (*Schinus terebinthifolia* Raddi); antioxidant activity; ultrasonic extraction

Science Projects for Students Showcase (SS-P-085)

Natural materials for wastewater purification

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Oil contamination in water sources significantly impacts the environment, economy, and public health both in Thailand and worldwide. Major causes include oil spills from tankers, industrial discharges, and wastewater release from communities. This study aims to develop a simple oil filtration system using agricultural and consumer waste materials, namely charcoal, coffee grounds, sawdust, rice husks, and rice straw. An oil-contaminated water simulation was created in a classroom setting, and the filtration was tested using recycled plastic bottles and a base layer of coarse sand. The efficiency of each natural material in absorbing oil was compared within a 5-minute filtration period. The results indicated that coffee grounds demonstrated the highest oil absorption, followed by charcoal, rice husks, rice straw, and sawdust, respectively. This study highlights the potential of utilizing waste materials to effectively address oil pollution in water sources, offering an environmentally friendly solution and promoting the sustainable use of resources.

Keywords: wastewater; natural; materials; watertreatment; coffee grounds; rice straw

Innovative natural absorbent and filtration materials for wastewater treatment

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This research investigates the use of agricultural waste materials, namely rice straw, coconut husk, and eggshells, for wastewater adsorption and filtration. Good water quality is defined by clarity and a pH range of 5.5-7 The study involves 4 main steps: 1.Preparation of an indicator kit from butterfly pea extract to indicate acid-base conditions. 2.Preparation of simulated wastewater to mimic real wastewater.3.Preparation of adsorbent materials by cutting them into small pieces and drying them to remove moisture.4.Testing the efficiency by mixing the adsorbent materials with wastewater for 10 minutes and filtering with Whatman No. 93 filter paper, followed by comparing turbidity and pH to evaluate the effectiveness.The experimental results showed that the adsorption effectiveness was highest for rice straw, followed by coconut husk and then eggshells. Rice straw demonstrated the best efficiency in adsorbing oil and filtering soil. After treatment, it could shift the pH from 7.9–8.4 to 6.6–7.3. Furthermore, it had the lowest cost at 50 baht/kg. These natural materials offer a sustainable alternative for future wastewater management that is practical and serves as a model for simple, low-cost, and environmentally friendly filtration, as well as a good option for utilizing limited resources.

Keywords: wastewater; natural materials; adsorption; rice straw; water treatment

Science Projects for Students Showcase (SS-P-087)

Low-cost adsorbent derived from banana stalk for removal of methylene blue from aqueous solution

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This research aims to utilize agricultural waste, specifically banana stalks, as a low-cost and natural adsorbent for removal of methylene blue, cationic dye commonly used in the textile industry. Banana stalks, as an abundant agricultural waste, along with the porous structure and cellulose content in banana stalks, significantly contribute to the potential for dye adsorption. In preparation, the banana stalks were cut into small pieces, sun-dried for one day, ground into a fine powder, and sieved to achieve uniform particle size. The adsorption efficiency was studied using batch system. The optimal adsorbent dosage was investigated in the range of 2.0 to 20.0 g/L. The results indicated that the most effective adsorbent dosage was 2.0 g/L for a contact time of 24 hours, an initial methylene blue concentration of 100 mg/L, achieving a high removal efficiency of 98.10%. The important findings of this research are that it enhances the low-cost preparation of adsorbents from inexpensive materials. This method is effective and holds significant application potential. Moreover, it provides an efficient way to recycle biomass waste, aligning well with the principles of the Bio-Circular-Green economy.

Keywords: banana stalks; agricultural waste; adsorption; methylene blue; bio-circular-green economy

Science Projects for Students Showcase (SS-P-088)

The study of biosensors from electrical graphs obtained from the cultivation of mycelium on agar mixed with sodium chloride in *Schizophyllum commune* and *Lentinus squarrosulus*

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It has been discovered that mushrooms can generate electrical activity to communicate within mushrooms in the same ecosystem, similar to the human nervous system but much less complex. The electrical activity of the mushrooms can be represented in the form of graphs. Additionally, the graphs can change in response to stimuli the mushrooms receive. This project was carried out to study the graphs obtained from the response to sodium chloride of two types of mushrooms: *Schizophyllum commune* and *Lentinus squarrosulus*, as they are local mushrooms in Thailand. The experiment was grew mycelium in regular Petri dishes and dishes mixed with sodium chloride. Electrical currents were recorded using an oscilloscope, and the data were presented in graph form to analyze the patterns of the graphs from mycelium grown in Petri dishes mixed with sodium chloride and compared to those grown in regular dishes. The graphs from different mushroom species follow the same pattern across all mushroom types. The results showed that the three mushroom types grown in petri dishes with high sodium chloride content resulted in higher peak values on the graphs. *Schizophyllum commune* and *Lentinus squarrosulus* species had slightly different peak values, with the highest peak ranging between 72-75 millivolts.

Keywords: mushroom; peak; graphs; oscilloscope; sodium chloride

Science Projects for Students Showcase (SS-P-089)

Utilization of banana stem as a sustainable and low-cost adsorbent for adsorption of brilliant green from aqueous solutions

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Banana stem, a readily available and underutilized agricultural residue, was explored as a sustainable, low-cost adsorbent for the treatment of effluents. Textile effluents often contain synthetic dyes, such as brilliant green, which pose serious environmental hazards. This study investigates banana stem waste as an adsorbent for removing brilliant green. The banana stem's porous structure and high cellulose content play a key role in its dye adsorption efficiency. Banana stems were chopped, sun-dried for 1-2 days, ground, and sieved to obtain uniform particles for adsorption studies. Batch adsorption experiments were conducted with dosages ranging from 2.0 to 20.0 g/L, at a contact time of 24 hours, and an initial dye concentration of 100 mg/L. The optimal dosage was determined to be 2.0 g/L, providing a high dye removal efficiency of 95.88%. The results confirm the potential of banana stem as an effective and eco-friendly adsorbent for dye-contaminated wastewater treatment. This work also supports sustainable waste management, contributing to the Bio-Circular-Green economy model by promoting circular economy practices.

Keywords: banana stem; agricultural residue; adsorption; brilliant green; bio-circular-green economy

Science Projects for Students Showcase (SS-P-090)

Effective cationic dye removal from aqueous solution using banana peel waste as a low-cost and eco-friendly adsorbent

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This research focuses on the use of agricultural biomass waste, specifically banana peels, for removing malachite green dye, a cationic industrial dye commonly producing pollutant in textile effluents. Banana peel possesses a porous structure and contains cellulose components, which play a significant role in its dye adsorption performance. Banana peel is a widely available and low-cost material with promising adsorption capabilities. To prepare the adsorbent, banana peels were chopped into small segments, sun-dried for 1 day, finely ground, and sieved to obtain particles of consistent size. Batch adsorption experiments were conducted to assess removal efficiency, with adsorbent dosages ranging from 2.0 to 20.0 g/L, a contact time of 24 hours, and an initial dye concentration of 100 mg/L. The results show that an adsorbent dosage of 4.0 g/L results in high removal efficiency of 96.90%. Accordingly, banana peel waste could be successfully used as a highly effective adsorbent for the treatment of malachite green dye in wastewater in the future. Furthermore, this work supports sustainable waste management and corresponds to the principles of the Bio-Circular-Green economy model.

Keywords: banana peel; agricultural biomass waste; adsorption; malachite green; bio-circular-green economy

Egg trays application as eco-friendly adsorbents for removal of brilliant green from aqueous solution

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This study investigated the utilization of egg tray waste, commonly discarded in communities, as low-cost adsorbents by the adsorption of brilliant green, an industrial cationic dye. Egg trays, primarily made of cellulose pulp, feature a porous structure that makes them highly suitable for adsorption applications. The adsorbent was prepared by cutting the egg trays into small pices, soaked in water for 1 day before grinding. The mixtures were then filtered through the cloth filter. The residues were oven-dried at 80ºC for 16 hours. Batch adsorption experiments were conducted with adsorbent dosages ranging from 2.0 to 20.0 g/L, at a contact time ranging from 1 hour to 24 hours, with an initial dye concentration of 100 mg/L. The results show that the optimal adsorbent dosage is 2.0 g/L with contact time of 6 hours providing dye removal efficiency of 97.1%. These findings demonstrate that egg trays are alternative effective sustainable and low-cost adsorbents offering a practical solution for dye removal, meanwhile adding value to community waste.

Keywords: egg trays; adsorbents; brilliant green

Science Projects for Students Showcase (SS-P-092)

Utilization of corn cobs as an eco-friendly adsorbent for industrial dye adsorption from aqueous solutions

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Saisamorn Lumlong,[3] Pornpan Pungpo[3,*]
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Corn cobs, an abundant agricultural by-product generated post-harvest, are often disposed of through open burning, contributing to air pollution. To address this environmental concern and promote sustainable waste management, this research aims to utilize corn cobs as an economic adsorbent for treating synthetic wastewater from industrial dye. Due to their porous cellulose structure, corn cobs were utilized to adsorb methylene blue, an industrial dye widely used in the textile industry, from aqueous solutions. Corn cobs were chopped, oven-dried at 80 ºC for 16 hour, ground, and sieved to obtain uniform particles for adsorption experiments. Batch adsorption experiments were conducted. To determine optimal parameters for adsorption process, adsorbent dosage and contact time were considered with adsorbent dosages ranging from 2.0 to 20.0 g/L and contact time ranging from 1 hour to 24 hours. The synthetic dye wastewater was prepared at the initial dye concentration of 100 mg/L. The results indicated that the optimal corn cob dosages for methylene blue adsorption is 10.0 g/L with corresponding optimal contact times of 3 hours. Under these optimum conditions, the removal efficiencies achieved was 96.7%. These findings demonstrate that corn cobs successfully serve as an effective and eco-friendly adsorbent, offering a valuable approach to repurposing agricultural waste in alignment with the Bio-Circular-Green economy.

Keywords: corn cobs; adsorption; methylene blue; agricultural by-product utilization

Science Projects for Students Showcase (SS-P-093)

Chitin and chitosan from 17-year-awaited cicada slough: Extraction and preparation

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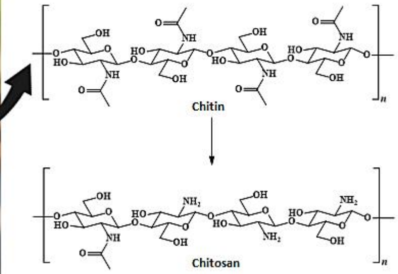
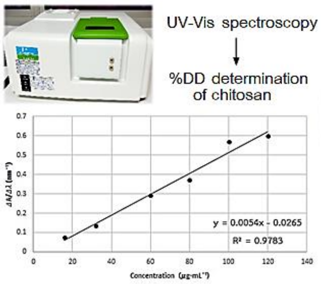
This project aimed to investigate the chitin extraction and chitosan preparation from cicada slough. Initially, chitin extraction was performed by grinding the cicada slough into power, followed by demineralization with 1 M HCl and deproteinization with 1M NaOH, respectively. The resulting chitin was subsequently bleached with NaOCl solution yielding 48% of chitin power. While chitosan was prepared by deacetylation reaction under chemical conditions, e.g. stirring in 40% NaOH at room temperature, refluxing in 40% NaOH, and refluxing in 60% NaOH solutions. A calibration curve of standardized GlcNAc solutions constructed by using UV-Vis spectroscopy was applied to determine the degree of deacetylation (%DD) of the prepared chitosan. Characterization of both chitin and chitosan from cicada were performed by using ART-FTIR spectroscopy. It was found that the highest deacetylation, 77.35%DD, of chitin was obtained under refluxing in 60% NaOH. Additionally, chitosan film was successfully prepared by dissolving chitosan in 2% acetic acid and glycerol. The present study could demonstrate the potential of cicada slough as alternative and sustainable resource for chitosan production and biopolymer materials.

Keywords: chitin; chitosan; cicada slough






Chitosan film

Science Projects for Students Showcase (SS-P-094)

Development of an adsorption-based oil separator for oil-contaminated sand using adsorbent materials and silica aerogel

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Oil spills from drilling, transportation, and related activities pose significant environmental and public health hazards. Conventional remediation techniques, including sand washing and thermal evaporation, are often inefficient, labor-intensive, and costly. This study presents a hydrophobic material-based system for remediating oil-contaminated sand. Silica aerogel was synthesized from sodium silicate, acid, and hexane, hydrophobized with isopropyl alcohol (IPA) and trimethylchlorosilane (TMCS), and heat-treated at 150°C to produce a hydrophobic powder, which serves as the key factor for adsorbing oil from contaminated sand. Additionally, a sponge coated with 20% v/v Starguard FCS was incorporated to improve absorption efficiency and enable reuse after compression. The system operated by spinning oil-contaminated sand with the absorbents. Upon water addition, oil-saturated aerogel and sponge floated and were collected by sweeping into a collection box. The independent variable was the mass of silica aerogel (1.35-2.70 g), while the dependent variable was the oil absorption percentage. Controlled variables included sand mass (30 g), oil volume (4 mL or 1.8 g), and sponge quantity. The optimal ratio of 17:1:1.5 (sand:oil:aerogel) achieved 93.33% oil removal efficiency, demonstrating a rapid, reusable, and effective remediation solution.

Keywords: oil-contaminated sand; silica aerogel; adsorption; hydrophobic

Science Projects for Students Showcase (SS-P-095)

Efficacy of clove extract in controlling the growth of *Bipolaris oryzae* the causal agent of brown leaf spot in rice fields

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Thailand's rice exports have declined over the past five years due to brown spot disease caused by *Bipolaris oryzae.* Farmers typically use chemical fungicides, which have negative effects on both the environment and human health. This study focuses on using clove (*Syzygium aromaticum*) extract for fungal control. The essential oil was extracted using steam distillation, and the minimum inhibitory concentration (MIC) was tested both in petri dishes and under natural conditions. The extraction yielded 10.82% (w/w) essential oil, and a gas chromatography-mass spectrometry analysis confirming 78.17% eugenol content. The MIC values were assessed at concentrations of 5, 10, 20, 40, 60, and 80 ppm over 24, 48, 72, and 96 hours. The lowest concentration that completely inhibited fungal growth was 10 ppm, achieving 100% inhibition compared to the control, which exhibited an average fungal growth diameter of 11.43 mm/24 h. Antifungal efficacy tests in petri dishes showed that clove extract and eugenol can inhibit growth well when compared to ethanol and control sets with inhibition percentages of 100.00, 100.00, 4.65 and 0.00, respectively. Disease resistance assessment using the Sutiwanich (1989) scoring system recorded disease severity scores of 0, 0, and 3 for clove extract, 95% ethanol, and the control, respectively.

Keywords: rice; brown spot disease; *Bipolaris oryzae*; clove; plant extracts

Science Projects for Students Showcase (SS-P-096)

Comparison of lead adsorption efficiency in wastewater using shells of river snail, green mussel, and blood cockle

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This project aims to compare the lead (Pb) adsorption efficiency of three types of Mollusk shell: Shells of river snail, green mussel, and blood cockle were dried at 100 °C for 4 h, calcined at 550 °C for 4 h, ground, and sieved to 40-mesh powder. Adsorption tests were carried out by adding 1.0 g of each powder to 100 mL of $Pb(NO_3)_2$ solution (initial $[Pb^{2+}] = 23.49 \pm 0.44$ mg/L), shaken at 200 rpm for 1 h. Residual Pb^{2+} concentrations measured by ICP-OES decreased to 0.092 ± 0.005 mg/L (river snail), 0.561 ± 0.009 mg/L (green mussel), and 0.725 ± 0.014 mg/L (blood cockle). All three powders effectively removed Pb(II), with river snail shell showing the highest efficiency—likely due to its higher calcite content and more porous surface enhancing ion binding.

Keywords: adsorbent material; adsorption efficiency; precipitation

Science Projects for Students Showcase (SS-P-097)

Structural and morphological characterization of chemical gardens formed from binary salt mixtures

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Chemical gardens are precipitations formed by metal ions that self-organize into complex structures resembling biological growth. This study investigates the formation of chemical gardens from two metal salts, $CuSO_4$ and $CoCl_2$, injected sequentially into a Hele-Shaw cell containing a sodium silicate (Na_2SiO_3) matrix. The resulting patterns were recorded as videos, and then the total areas of the pattern, growth rates, and pattern densities were analyzed. By varying flow rates, morphological analysis of precipitates revealed four distinct types: filaments, worms, hairs and a newly observed type “feather”. The feather-like pattern radiates outwards from the cracks of pre-existing structures, resembling the plumulaceous barbs of a feather, which is an uncharacteristic feather compared to previously observed patterns. When both salts were combined, the precipitates more closely resembled those of the initial salt solution (copper in this study). Furthermore, the pattern types formed by the two salts influenced the growth rate, with the combined salts exhibiting a higher growth rate than the individual salts, suggesting a collaborative growth mechanism.

Keywords: chemical gardens; Hele-Shaw cell; precipitation; patterns; collaborative growth

Future Chemistry Research Presentation for Undergraduate Students (US-P-001)

Magnetic $CoFe_2O_4$/MIL-53/carbon aerogel composite for efficient organic dye adsorption in wastewater treatment

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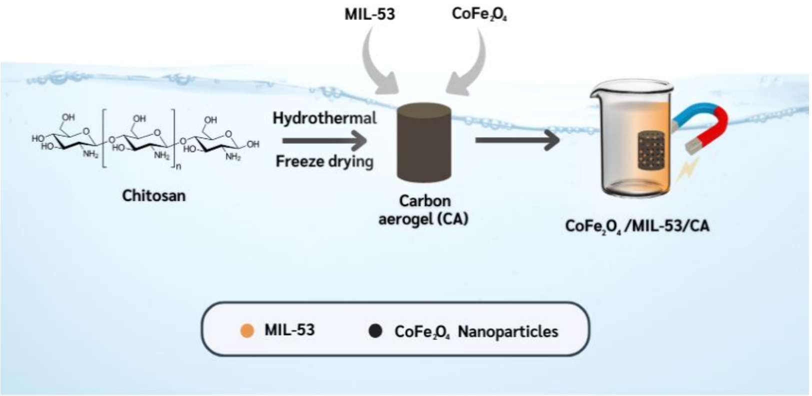
Dye adsorption using nanocomposites has emerged as a highly effective and sustainable approach for the removal of organic dyes from wastewater, addressing the critical issue of water pollution and ensuring environmental safety through enhanced adsorption capacity, selectivity, and reusability. In this study, magnetic $CoFe_2O_4$ nanoparticles supported on biomass-derived carbon aerogels (CA) from chitosan and metal-organic framework (MIL-53)-based aerogels were synthesized using a simple hydrothermal process. The obtained $CoFe_2O_4$/MIL-53/CA composites are lightweight, low-density, cost-effective, eco-friendly, and easily collected after the adsorption process. The structural, morphological, and physicochemical properties of the synthesized $CoFe_2O_4$/MIL-53/CA composites were characterized using Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), nitrogen (N_2) adsorption-desorption analyses, and transmission electron microscopy (TEM). The adsorption performance of the $CoFe_2O_4$/MIL-53/CA composite was evaluated for both cationic and anionic dyes. The $CoFe_2O_4$/MIL-53/CA composite exhibited superior adsorption properties compared to pristine $CoFe_2O_4$, MIL-53, and CA materials. This study introduces a novel $CoFe_2O_4$/MIL-53/CA composite with enhanced adsorption efficiency, recyclability, and environmental sustainability. The synergistic combination of magnetic nanoparticles, MOF-based aerogels, and biomass-derived carbon aerogels results in a high-performance adsorbent, offering significant potential for practical wastewater treatment applications.

Keywords: MIL-53; carbon aerogel; $CoFe_2O_4$ NPs; aerogel; dyes adsorption



Future Chemistry Research Presentation for Undergraduate Students (US-P-002)

Sustainable carbon aerogel/graphene oxide composite for efficient dye removal from wastewater

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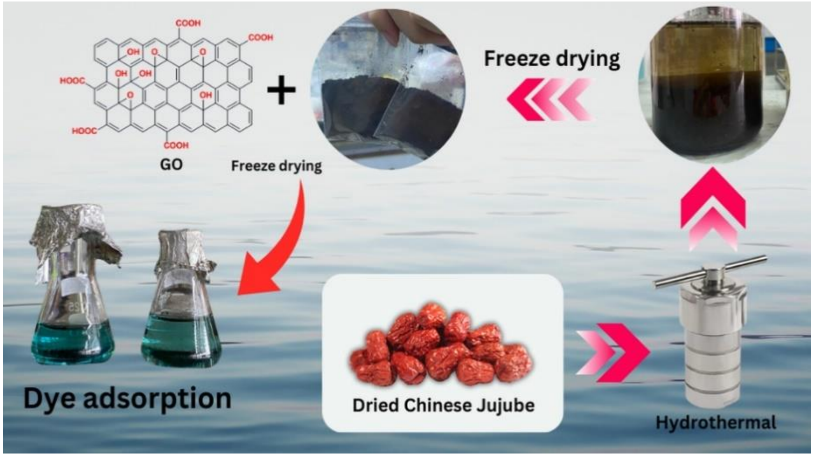
Water pollution caused by organic dyes is a significant environmental concern due to their toxicity, persistence, and resistance to degradation. Developing efficient, sustainable, and cost-effective adsorbents for dye removal is crucial for wastewater treatment. In this study, a composite of dried Chinese jujube-derived carbon aerogel and graphene oxide (CA-GO) was synthesized using a hydrothermal method followed by freeze-drying. The resulting CA-GO composites were characterized using XRD., FTIR, SEM/EDS, HRTEM and BET analysis. The adsorption efficiency of CA-GO and carbon aerogels was evaluated for both cationic and anionic dyes. The results indicated that CA-GO exhibited superior adsorption efficiency compared to carbon aerogel, primarily due to the enhanced surface properties imparted by graphene oxide. Additionally, the composite demonstrated a greater affinity for cationic dyes, such as Methylene Blue, compared to anionic dyes, such as Congo Red. This study highlights a sustainable and efficient approach to dye adsorption, with potential applications in wastewater treatment, energy storage, and biotechnology.

Keywords: carbon aerogel; graphene oxide; aerogel; surface sites; dye adsorption



Impact of electron beam irradiation on physicochemical properties of okara powder

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Okara, a nutrient-rich by-product, has limited use in food applications due to its undesirable physicochemical properties. This study investigated the impact of electron beam irradiation on okara powder to determine its potential for food use. The powder was irradiated at 0, 2.5, 5, and 7.5 kGy, and its chemical and physical properties were analyzed. Irradiation did not significantly affect moisture and protein content but led to a decrease ($p \leq 0.05$) in fat, crude fiber, and lightness (L^*), while increasing ΔE values, indicating noticeable color changes. Water holding capacity (WHC) decreased by 11.75%, whereas oil holding capacity (OHC) increased by 15.06%. The highest phenolic content (0.665 mg GAE/g) was observed at 5 kGy, though antioxidant activity declined. Scanning Electron Microscopy revealed increased porosity in irradiated samples. The observed changes in physicochemical properties provide insights into how electron beam irradiation influences okara powder, supporting its potential for use in food formulations.

Keywords: okara; electron beam; chemical properties; physical properties; nutritional

Click-chemistry-derived lipid nanoparticles for enhanced mRNA delivery

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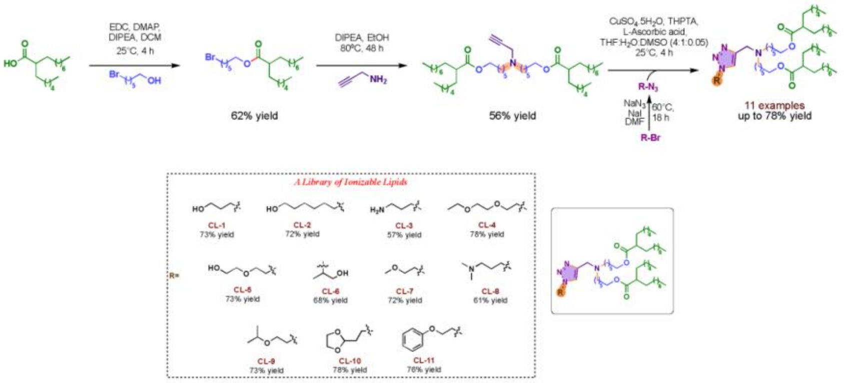
Lipid nanoparticles (LNPs) have emerged as a ground-breaking technology in the field of drug delivery, providing an efficient and adaptable platform for administering a broad spectrum of therapeutic agents, particularly nucleic acids. Among these, mRNA-based therapeutics have garnered significant attention, especially in the wake of the COVID-19 pandemic, underscoring the urgent need for rapid and effective delivery systems for mRNA. As a result, numerous research groups and pharmaceutical companies have devised various strategies for mRNA delivery, each aiming to optimize the efficiency and safety of mRNA-based treatments. While various strategies have been developed to optimize mRNA delivery, existing methods often suffer from low synthetic yields, lengthy reaction times, and high material consumption. To address these challenges, our team has focused on the strategic design and development of LNPs to enhance mRNA delivery. Specifically, we have devised a mild, efficient, and time-saving strategy to synthesize the ionizable lipid ALC-0315, a key component in commercial mRNA vaccines. This approach was further expanded to generate a diverse range of ionizable lipids using Click chemistry, introducing modifications in the hydrophilic head groups to optimize performance. By streamlining the synthetic process and improving scalability, our method offers a cost-effective alternative for pharmaceutical applications. *In vitro* and *in vivo* studies demonstrated superior or comparable nanoluciferase expression and encapsulation efficiency of our synthesized lipids compared to commercialized counterparts such as ALC-0315 (Pfizer-BioNTech) and SM-102 (Moderna). These findings highlight the feasibility of rational lipid design using click chemistry to generate highly efficient mRNA delivery systems. Our approach offers a promising pathway for developing next-generation LNPs with enhanced biocompatibility, encapsulation efficiency, and mRNA delivering capabilities.

Keywords: lipid nanoparticles (LNPs); mRNA delivery; ionizable lipids; Click chemistry; encapsulation efficiency



Strain-enabled radical spirocyclization: A modular approach to spirocyclobutyl sultams

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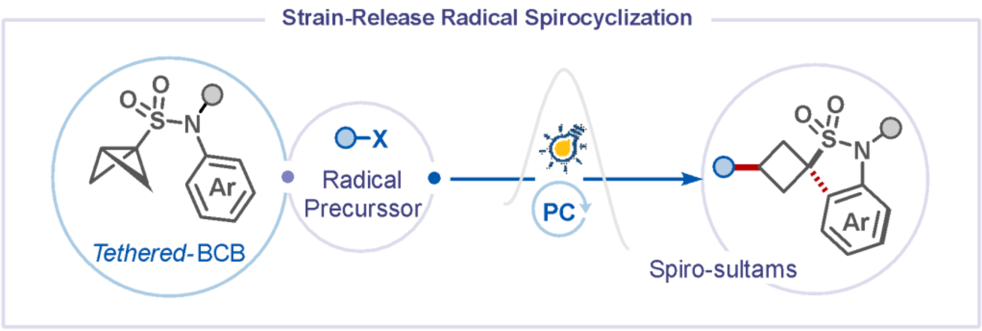
Sulfonamides have played a crucial role in medicinal chemistry and drug discovery. Sultams, the cyclic analogs of sulfonamides, are particularly noteworthy due to their enhanced biological activity and selectivity. Among these, the synthesis of spirocyclobutyl sultams remains largely unexplored, despite their potential in drug discovery. The incorporation of a cyclobutane ring not only enables precise spatial orientation of substituents along pre-defined vectors but also improves key physicochemical properties and pharmacokinetics. Herein, we report a novel photoredox-catalyzed strain-release radical spirocyclization strategy for the efficient synthesis of a library of functionalized spirocyclobutyl sultams. A diverse range of radicals, including thiotrifluoromethyl, sulfonyl, and phosphonyl groups, were successfully added to the strained C–C σ-bond of bicyclobutanes (BCBs), affording a structurally diverse library of spirocyclobutyl sultams. Overall, this modular and sustainable approach expands the chemical space of spirocyclic sultams and highlights their potential in the development of next-generation therapeutics.

Keywords: bicyclo[1.1.0]butane; strain-release; photoredox catalysis; spirosultams; spirocyclobutanes



Conversion of agricultural waste rice husks into silver nanoparticles as catalyst-evaluating their application in catalytic activity

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Rice is a staple food across Southeast Asia, producing vast amounts of rice husks (RH) as agricultural waste, often burned or discarded in landfills. Despite being rich in bioactive compounds, RH remain largely underutilized. Green synthesis of Silver Nanoparticles (AgNPs) using plant extracts has gained significant attention in the recent years. This study utilizes RH, to synthesize AgNPs for catalytic and photocatalytic applications. Para-nitrophenol (PNP), a toxic byproduct of industries like pharmaceuticals, often accumulates in water bodies, causing serious environmental and health risks. Similarly, azo dyes, such as methylene blue (MB) used in the textile industry, poses significant environmental and health hazards due to their toxic and carcinogenic nature. Conventional methods to degrade these toxic industrial wastes is expensive, slow and harnesses toxic byproducts, whereas AgNPs act as eco-friendly and highly effective alternative. The catalytic efficiency of AgNPs was demonstrated through the degradation of PNP using 4000 ppm AgNPs, causing an instant degradation. Additionally, the photocatalytic activity of AgNPs (4000 ppm and 266.67 ppm) was tested for the degradation of 1mM MB. Rapid degradation was observed, particularly at the lower concentration. These findings highlight the exceptional potential of eco-friendly AgNPs synthesized from RH for industrial applications in degrading harmful pollutants.

Keywords: silver nanoparticle; catalysis; photocatalysis; azo-dye; para-nitrophenol

Environment-friendly synthesis of silver nanoparticles using leaf extracts of mint (*Mentha*) and evaluation of their antioxidant activity

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Oxidative stress is caused by reactive oxygen species, which lead to an imbalance between oxidation and antioxidation. Natural antioxidants were produced by plants. This can be used to provide balance between oxidation and antioxidation. Five varieties Mint (*Mentha*) were used to produce silver nanoparticles (AgNPs) for natural antioxidant activity, such as Common mint (*Mentha*), Apple mint (*Mentha suaveolens*), Chocolate mint (*Mentha x piperita f. Citrata*), Spear mint (*Mentha spicata*) and Peppermint (*Mentha piperita*). Silver is used to synthesize nanoparticles and AgNPs synthesized by Eco-friendly biological method. This is non-toxic, economical and environment friendly. Plant extracts contain secondary metabolites which reduce the silver ions and generate the AgNPs. AgNPs were synthesized by optimization of temperature with different time periods. Four mint samples were produced nanoparticles at 90ºC for 60 minutes, which are: Common mint, Apple mint, Chocolate mint and Peppermint. AgNPs were observed under a scanning electron microscope for morphology analysis. Mint synthesized spherical shaped (40 nm) nanoparticles at 420 nm and all nanoparticles are semiconductors. Evaluate the total flavonoid content (TFC), total phenolic content (TPC) and total antioxidant capacity (TAC) and determine the correlation and coefficient between antioxidant activities of mint water extract and AgNPs samples. AgNPs samples have higher antioxidant activity than the water extract samples. The Pearson correlation and coefficient prove that there is a significant change between the water extract and AgNPs samples. TPC and TAC provide stronger correlations. Mint leaves contain higher phenols, and due to that, they can be used to treat free radical diseases.

Keywords: green synthesis; mint; AgNPs; antioxidant activity; correlation

Future Chemistry Research Presentation for Undergraduate Students (US-P-008)

Coconut (*Cocos nucifera*) husk extract mediated green synthesis of silver nanoparticles and evaluating its biological potential in terms of the antimicrobial, antioxidant and photocatalytic activity; A low-cost and an eco-friendly outlook

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Green synthesis of metal nanoparticles (NP) has become a promising synthetic strategy in nanotechnology. In this present study, the biosynthesis of silver nanoparticles (AgNPs) using five varieties of *Cocos nucifera* (coconut) husk extract is described. The influence of temperature variable was investigated to optimize the biosynthesis of AgNPs. The phytochemical screening of the husk extract proved the influence of phytochemicals in bio reduction, stabilization and capping process in nanoparticle synthesis. King coconut (KC) and Typica (TP) varieties involved in the biosynthetic process at 90ºC for 1 hour. The synthesized AgNPs were characterized by TEM and UV-visible spectrophotometric analysis. TEM images verified the presence of spherical AgNPs with the average size of 20nm which was further confirmed by the calculated band gap energies. Furthermore, TFC, TPC, TAC and DPPH assays analyzed the antioxidant potential where the results indicated a significant antioxidant potential in AgNPs compared to their water extracts. The synthesized AgNPs were found to be effective antimicrobial agents against *Staphylococcus aureus* and *Escherichia coli* compared to water extracts. The highest antimicrobial activity against *Staphylococcus aureus* and *Escherichia coli* was shown by KC AgNPs among the synthesized nanoparticles with a zone of inhibition of 2.5 cm and 2.7 cm respectively. The photocatalytic activity of 100ppm KC AgNPs for the degradation of malachite green dye under direct sunlight in the presence of $NaBH_4$ catalyst happened faster within 40 min compared to the degradation of dye in the absence of catalyst which took 2-hours. All the AgNPs were classified as semiconductors based on the calculated bandgap energies. Moreover, the present study is an attempt to utilize agricultural waste and is the first report for coconut husk assisted synthesis of AgNPs in Sri Lanka. Thus, it can be concluded that coconut husk extract is an ecofriendly source that can used extensively in the green synthesis of potent antioxidants, antimicrobial and photocatalytic AgNPs for commercial applications.

Keywords: *Cocos nucifera*; AgNPs; antioxidant activity; antimicrobial; photocatalysis

Future Chemistry Research Presentation for Undergraduate Students (US-P-009)

Synthesis of silver nanoparticles using aqueous extract of *Solanum lycopersicum* fresh leaves and analysis of antioxidant properties

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Green synthesis of nanoparticles has become a promising substitute to conventional chemical and physical nanofabrication methods mostly due to environmental-friendliness and cost effectiveness. Silver nanoparticles (AgNPs) out of other nanoparticles hold significance due to their high antioxidant and non-toxic nature making them ideal for various biomedical applications. The current study employed a rapid, simple approach for green synthesis of AgNPs using aqueous leaf extracts from five varieties of *Solanum lycopersicum* and were characterized using spectroscopic analysis in which surface plasmon resonance was detected within 400-500nm. This was visually confirmed by the colour change. They were subjected to TFC, TPC and TAC to evaluate antioxidant properties and statistical analysis was carried out. Scanning Electron Microscopic (SEM) analysis was performed to characterize the AgNPs. Maximum number of samples produced AgNPs under 60ºC for 45min. SEM images showed that AgNPs were spherical and 40nm in diameter. Based on bandgap energy, synthesized AgNPs were classified as superconductors as all bandgaps were <3eV. Higher TFC, TPC and TAC values were obtained for AgNPs compared to their respective water extracts, thus indicating that AgNPs had higher antioxidant activity. Statistical analysis distinguished strong positive correlations between TAC-TPC, TAC-TFC and TPC-TFC antioxidant assays. In conclusion, the AgNPs synthesized using aqueous *Solanum lycopersicum* leaf extracts could be used as promising therapeutic molecules with significant antioxidant activities, thus can be used in diverse applications due to its eco-friendly, cost-effective and reproducible nature.

Keywords: green synthesis; *Solanum lycopersicum*; AgNPs; antioxidant activity

Future Chemistry Research Presentation for Undergraduate Students (US-P-010)

Green synthesis of silver nanoparticles using *Caesalpinia pulcherrima* flower extracts: Evaluating their antibacterial, antioxidant and photocatalytic activity

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The contemporary advancement of nanobiotechnology, where nanoparticles are green synthesised using biological bottom-up approach to overcome the limitations of conventional methods has gained attention in numerous fields, including medicine. This study aimed to green synthesize silver nanoparticles (AgNPs) using five varieties of *Caesalpinia pulcherrima* (CP) (Orange, Yellow, Red, Pink Yellow and Pink) in an environmentally friendly and sustainable approach and determine their antioxidant, photocatalytic and antibacterial properties. The AgNPs were synthesised at optimum temperature at 90 °C for 60 minutes and were characterized using UV-visible spectrum, that showed a plasmon resonance peak between 400-460 nm. Transmission electron microscopy analysis revealed the synthesised CP AgNPs are spherical in shape and 20 nm in size. AgNPs are classified as semiconductors based on their bandgap energy of 2.82 eV and 2.95 eV. Antioxidant properties were evaluated by total flavonoid content (TFC), total phenolic content (TPC), total antioxidant capacity (TAC) and DPPH free radical scavenging assays – which revealed that AgNPs has higher antioxidant properties than water extracts. Photocatalytic activity of CP AgNPs was assessed using Methylene blue (MB), which showed that 100 ppm and 500 ppm AgNPs degrade MB within 24 hours both in presence and absence of $NaBH_4$ catalyst. Antibacterial activity of CP AgNPs against *E. coli* and *S. aureus* showed no significant difference in comparison to their water extracts. The biosynthesized AgNPs could be used in treating free radical-mediated diseases and multidrug resistant bacterial infections and minimize environmental pollution by degrading organic dyes to non-toxic intermediate compounds.

Keywords: *Caesalpinia pulcherrima*; AgNPs; antioxidant activity; antimicrobial; photocatalysis

Determination of antioxidants properties of silver nanoparticles using *Solanum melongena* extract

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Bio nanotechnology is a combination of biotechnology and nanotechnology that aims to build biosynthetic and environmentally friendly nanomaterial synthesis technologies. The use of a green approach to synthesize various metallic nanoparticles has recently attracted a lot of attention among scientists. Nature's capacity to break down metallic ions into their constituent nanoparticles has been discovered during the search seeking new plant-based lowering and/or capping substances. Because nanomaterials are much smaller than most biomolecules and structures, they can be used in both in-vitro and in vivo biomedical studies. Silver nanoparticles (AgNPs) have gained great importance due to their high antioxidants, antimicrobial, non-toxic nature and biological functionality which make them ideal for biomedical applications. The present study describes the green synthesis of silver nanoparticles (AgNPs) using leaf aqueous extract of five *Solanum* species (*Solanum melongena, Solanum torvum, Solanum incanum, Solanum procumbens, Solanum xanthocarpum)*. The synthesized AgNPs were characterized using, UV-vis spectrum which shows a Plasmon resonance peak between 350 – 400 nm. It was able to identify higher antioxidant properties in AgNPs than in water extracts. Afterwards the total phenolic content and total antioxidant capacity, total flavonoid content was determined by the Gallic acid standard curve, Ascorbic acid standard curve and Quercetin standard curve respectively. The spherical nanoparticles in this SEM image were found to be in the size of 40 nm with a morphological diversity. Thereby, green synthesized AgNPs from *Solanum* species could be used in medical research to reduce free radical induced diseases.

Keywords: silver nanoparticle; *Solanum melongena*; antioxidant; phenols; flavanols

An eco-friendly approach for the green synthesis of silver nanoparticles using *Petunia* leaf extracts and assessing their antibacterial, antioxidant and photocatalytic activity

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Recent advances in nanotechnology have resulted in limitless applications of nanomaterials, an important role in medicine is one such application. Silver nanoparticles (AgNPs) have gained popularity, as it is ideal for biomedical applications due to their high antioxidant, antibacterial, biological functionality and non-toxicity. This study describes the antioxidant, photocatalytic and antibacterial activity of AgNPs synthesized using five different *Petunia hybrida* leaf extracts (black, white, pink, purple, pink-purple) for the first time. Initially, the colour change indicated the presence of produced AgNPs. UV-Vis spectroscopy and transmission electron microscopy (TEM) were used to analyse the formation, size, and shape of the produced AgNPs. The bandgap energy and TEM image of pink AgNPs indicated that the synthesized AgNPs were in the 50 nm range. The existence of phytocompounds was identified by qualitative phytochemical analysis. Carbohydrates, terpenoids and steroids were found in all *Petunia* samples. TFC, TPC, TAC, DPPH and IC_{50} tests were used to assess the antioxidant activity of leaf water extracts and AgNPs. The antioxidant assay findings demonstrated that AgNPs had stronger antioxidant activity than their respective leaf water extracts. The agar well diffusion technique revealed that the produced AgNPs had significant antibacterial activity against *Escherichia coli* compared to *Staphylococcus aureus*. Moreover, the photocatalytic activity of the produced pink-purple AgNPs at 100 ppm was investigated by removing malachite green dye from an aqueous solution under sunlight in the presence and absence of $NaBH_4$ catalyst. In 40 minutes, 100 ppm pink-purple AgNPs demonstrated effective photocatalytic activity in the breakdown of malachite green. The findings suggested that *Petunia* is an eco-friendly source for AgNP biosynthesis, which can be employed as a novel antioxidant, antibacterial, and photocatalytic agent; hence, it may be used in a range of applications to contribute to a better life.

Keywords: *Petunia* leaf; AgNPs; antioxidant activity; antimicrobial; photocatalysis

Future Chemistry Research Presentation for Undergraduate Students (US-P-013)

Chitosan-stabilized silver nanoparticles: An investigation into their predicted stability through molecular dynamic simulations and *in silico* toxicity analysis

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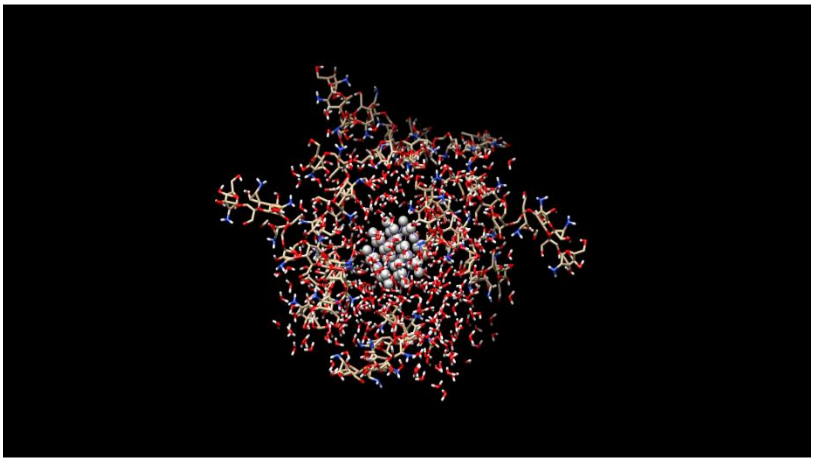
Silver nanoparticles (AgNPs) are a major advancement in nanomedicine, known for their antimicrobial and anti-cancer properties. Their stability is crucial for effectiveness, often enhanced by stabilizers like chitosan. Computational methods were used to assess the stability and toxicity of chitosan-stabilized silver nanoparticles (CS-AgNPs). AgNPs structure was designed using CHARM GUI interface, while chitosan polymer was optimized using DFT with basis set 6-311++g(d,p). Molecular docking investigations revealed a weak non-bonding interaction (+0.03 kcal/mol) between the silver atom and chitosan. Molecular dynamics simulations showed that AgNPs are unstable without chitosan, evident by significant fluctuations in the Radius of gyration (Rg) and Root Mean Square Deviation (RMSD). In contrast, AgNPs within chitosan exhibited stable Rg and minimal RMSD increase. The toxicity of the CS-AgNPs was predicted using the ProTox-3.0 web tool. Predictions of toxicity revealed that uncoated AgNPs showed neurotoxicity (0.59), high permeability across the blood-brain barrier (0.99), and ecotoxicity (0.78), all of which were significantly improved by chitosan coating. CS-AgNPs exhibited enhanced biocompatibility due to reduced interaction with CYP2C9 and lower mutagenicity, MD simulations emphasizing the efficacy of chitosan in stabilizing AgNPs and lessening their potential toxicity, thereby increasing their safety for both biomedical and environmental applications.

Keywords: chitosan; silver nanoparticles; molecular docking; molecular dynamics; toxicity



Future Chemistry Research Presentation for Undergraduate Students (US-P-014)

Photocatalytic degradation of tetracycline development of a magnetic $MnFe_2O_4$/biochar photocatalyst for sustainable antibiotic removal from wastewater

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This study presents the synthesis of manganese ferrite ($MnFe_2O_4$) and its composite with duckweed-derived biochar ($MnFe_2O_4$/BC) as photocatalysts for tetracycline (TC) degradation under low-intensity UV light. $MnFe_2O_4$, known for its chemical stability, magnetic properties, and UV responsiveness, was synthesized using co-precipitation and hydrothermal methods. To enhance photocatalytic efficiency, $MnFe_2O_4$ was integrated with biochar produced from Lemna minor, a fast-growing aquatic plant with high surface area and adsorption capacity. The $MnFe_2O_4$/BC composite synergistically combines adsorption and photocatalytic degradation, promoting improved charge separation and pollutant removal. Photocatalytic experiments confirmed that $MnFe_2O_4$/BC demonstrated superior TC degradation efficiency compared to $MnFe_2O_4$ alone, under energy-efficient UV conditions. The magnetic recoverability of the catalyst and the use of renewable duckweed-based biochar further support its environmental and practical viability. This work highlights a green, low-cost, and effective approach for antibiotic removal from wastewater, contributing to the development of eco-friendly and reusable materials for water purification applications.

Keywords: manganese ferrite; biochar; tetracycline degradation; photocatalysis; wastewater treatment

Analysing the phytochemical and antioxidant profile of *Pandanus amaryllifolius* in response to different abiotic stress conditions

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Plant stress is a phenomenon in which plants develop in unfavourable environmental conditions causes by a range of biotic and abiotic factors. Stress can cause limitations in agriculture yields and growth, as well as permanent damage or death if it exceeds the thresholds of plant tolerance. *Pandanus amaryllifolius,* which belongs to the Pandanaceae family, is typically utilized in pharmaceutical and food additives industry as a source of bioactive chemicals, flavoring and natural coloring. Among the Pandanus species, *P. amaryllifolius* has distinctively fragrant leaves, which are ascribed to its main fragrance component, 2-acetyl-1-pyrroline (2AP). This study aimed to analyse the phytochemical and antioxidant profile of *Pandanus amaryllifolius* in response to different abiotic stress conditions such as, flood, high salinity, drought and nutrient deficiency. Quantitative tests such as total phenolic content (TPC), total flavonoid content (TFC), total antioxidant capacity (TAC) and total protein content (TPrC) were performed to analyse how *Pandanus amaryllifolius* responds to different abiotic stress conditions. TPC was determined using the Folin-Ciocalteu method, based on the reduction in the presence of phenolics, producing molybdenum-tungsten blue, which is detected spectrophotometrically at 760 nm. TFC was analyzed using Aluminium Chloride ($AlCl_3$) method. The idea behind in this method is that $AlCl_3$ combines with the C-4 keto groups and either the C-3 or C-5 hydroxyl groups of flavones and flavonols to produce acid-stable complexes. Additionally, it combines with the ortho-dihydroxyl groups in flavonoid rings to generate acid-labile complexes. TAC was determined using phosphomolbdate method, which is based on the principal behind that extract or a compound with antioxidant potential converts Mo(VI) to Mo(V), producing a green phosphate Mo(V) complex at an acidic pH. The Lowry method used to analysed TPrC is based on the reduction of F-C phosphotungtic and phosphomolybdic acid, followed by the reaction of the peptide nitrogen with the copper(II) ions in an alkaline environment. According to the results, *Pandanus amaryllifolius* under nutrient deficiency condition exhibited higher Total phenolic content (18.18 mgGAE/g), Total antioxidant capacity (21.72 mgAAE/g) and Total protein content (101.38 mgBSAE/g) values compared to control and other abiotic stress conditions. These findings suggest a stress-induced activation of the phenylpropanoid biosynthetic pathway, enhancing the production of hydroxylated aromatic compounds with antioxidant functions.

Keywords: *Pandanus amaryllifolius*; total phenol content; total flavonoid content; total antioxidant capacity; total protein content

Future Chemistry Research Presentation for Undergraduate Students (US-P-016)

Molecular weight distribution of bioactive sialylated-mucin (SiaMuc) glycopeptide recovered from edible bird's nest (EBN) by-product using enzymatic hydrolysis

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Edible bird's nest (EBN) is a dried secretion of salivary mucin produced by swiftlets during breeding and is highly valued for its nutritional benefits, particularly in Chinese communities across Southeast Asia. The labor-intensive cleaning process, which involves handpicking to remove inedible materials, generates about 30% by-product waste, mainly composed of feathers rich in mucin glycoproteins (~50%). Despite its potential, limited research has focused on recovering valuable components from these by-products. This study explores enzymatic hydrolysis to breakdown EBN by-products (EBN-BP) into bioactive glycopeptides and free peptides, facilitating the separation of inedible materials through ultrafiltration, while assessing its effect on physicochemical properties, molecular weight (MW) distribution, and glycopeptide integrity. Findings from the study revealed that the enzymatic recovery slightly reduced soluble protein (2.31±0.74%) and glycoprotein content (72.85±6.44%) in EBN-BP hydrolysate, while increasing peptide (64.40±8.84%) and reducing sugar content (31.18±1.45%). Molecular weight analysis showed similar glycoprotein (~11.8–163.8 kDa) and protein (~12.5–127.6 kDa) profiles in EBN-BP hydrolysate and cleaned EBN hydrolysate, with additional fractions likely from feathers. In conclusion, enzymatic recovery of bioactive SiaMuc-glycopeptide hydrolysate from EBN by-products maintains similar physicochemical properties and MW distribution. This approach offers an economical alternative for ESN, enhancing industrial use by reducing MW without compromising the quality of bioactive SiaMuc-glycoproteins.

Keywords: edible swiftlet's nest; SDS-PAGE; electrophoresis; EBN hydrolysate; EBN waste

Future Chemistry Research Presentation for Undergraduate Students (US-P-017)

One-pot hydrothermal synthesis of $BiVO_4/g\text{-}C_3N_4$ composite for efficient photocatalytic degradation of tetracycline

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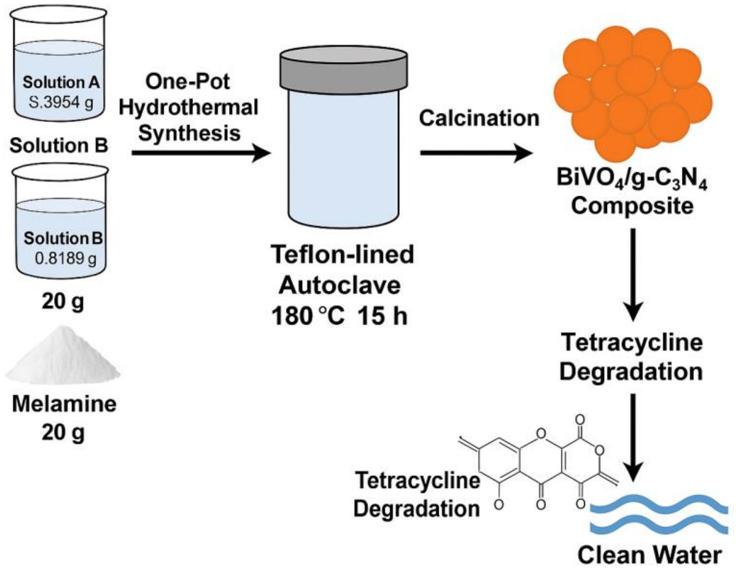
This study presents a one-pot hydrothermal synthesis approach for the fabrication of $BiVO_4/g\text{-}C_3N_4$ composite photocatalysts, designed for the efficient degradation of tetracycline in aqueous environments. $BiVO_4$ was synthesized by reacting $Bi(NO_3)_3{\cdot}5H_2O$ and NH_4VO_3 in acidic and basic media, respectively, followed by hydrothermal treatment at 180 °C for 15 hours and subsequent calcination at 500 °C. Separately, $g\text{-}C_3N_4$ was obtained from melamine under identical hydrothermal and thermal conditions. For the composite preparation, melamine powder was incorporated into the $BiVO_4$ precursor solution prior to hydrothermal treatment, facilitating in-situ formation of a $BiVO_4/g\text{-}C_3N_4$ heterojunction. The resulting photocatalysts were washed, dried, and thermally treated to ensure high crystallinity and structural stability. The $BiVO_4/g\text{-}C_3N_4$ composite synthesized via this green, scalable method exhibits promising potential for photocatalytic degradation of tetracycline under visible light, highlighting its relevance in addressing pharmaceutical contaminants in wastewater.

Keywords: one-pot hydrothermal synthesis; tetracycline degradation; photocatalysis; wastewater treatment



Future Chemistry Research Presentation for Undergraduate Students (US-P-018)

Low-intensity UV activated Cu-doped $BiVO_4$: Synergistic performance in organic pollutant removal and microbial inactivation

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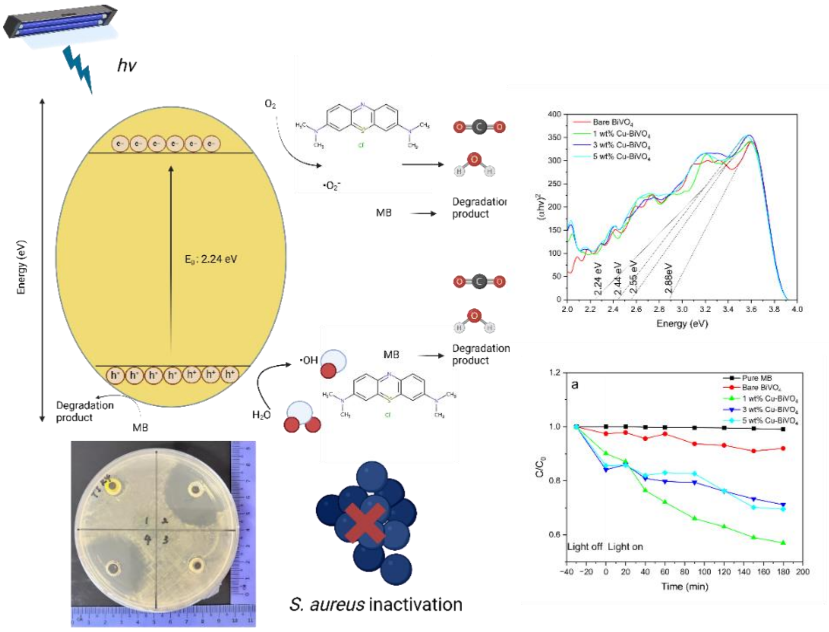
The textile industry discharges toxic dyes like methylene blue (MB) into water bodies, necessitating sustainable treatment solutions. Here, we report a dual-functional Cu-doped $BiVO_4$ photocatalyst synthesized via a scalable hydrothermal method. Optimized 1 wt% Cu doping narrowed the bandgap to 2.24 eV, enabling 85% MB degradation under low-intensity UV (13 W) within 180 minutes—a 5.1-fold enhancement over bare $BiVO_4$. Radical trapping confirmed hydroxyl radicals (•OH) and superoxide radicals ($•O_2^-$) as the dominant reactive species. The catalyst retained >92% efficiency over three cycles and exhibited antibacterial activity against *Staphylococcus aureus* (12.6 ± 0.4 mm inhibition zone) in dark conditions, attributed to Cu^{2+} release. Cost analysis further revealed a competitive synthesis cost of approximately RM 7.57 per gram, supporting the economic viability for large-scale environmental remediation applications. The dual photocatalytic and antibacterial functionalities, combined with cost efficiency, underscore the practical applicability of Cu-doped $BiVO_4$ for wastewater treatment.

Keywords: bismuth vanadate; copper doping; hydrothermal; photocatalysis; antibacterial; methylene blue



Future Chemistry Research Presentation for Undergraduate Students (US-P-019)

Evaluation of ZIF-8/graphene composite for low-intensity UV-driven levofloxacin degradation and antibacterial activity

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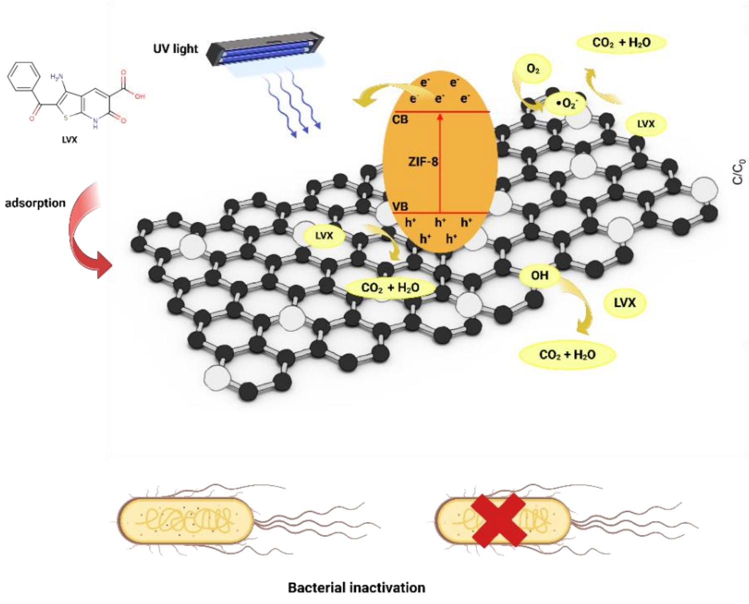
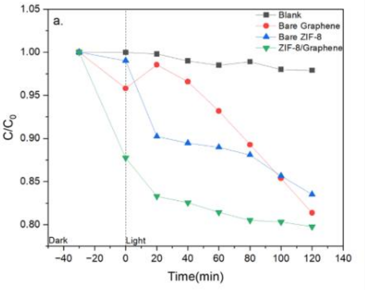
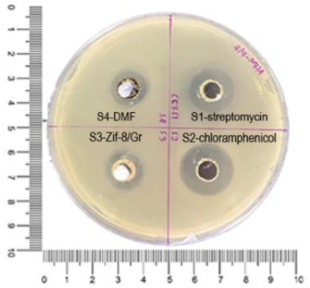
In this study, we synthesized a ZIF-8/graphene (Gr) composite and evaluated its photocatalytic degradation performance toward levofloxacin (LVX) under low-intensity UV light. The composite exhibited improved charge separation and enhanced reactive oxygen species (•OH, $•O_2^-$, h^+) generation compared to its individual components. Under optimal conditions (20 mg catalyst, 5 mg/L LVX, neutral pH), a 25.70% degradation was achieved after 120 minutes of irradiation, following pseudo-first-order (PFO) kinetics. While the degradation efficiency was modest, the catalyst operated effectively under low-energy conditions and demonstrated selective antibacterial activity against *E. coli* in dark conditions. The findings suggest that ZIF-8/Gr composites hold potential as dual-functional materials for pollutant attenuation and microbial control in niche wastewater applications, particularly where energy constraints are critical. Further work is needed to enhance degradation efficiency and assess long-term operational stability.

Keywords: photocatalyst; antibiotics; ZIF-8; graphene; reactive species







Future Chemistry Research Presentation for Undergraduate Students (US-P-020)

Facile hydrothermal conversion of duckweed into NH_2-functionalized biochar for water treatment applications

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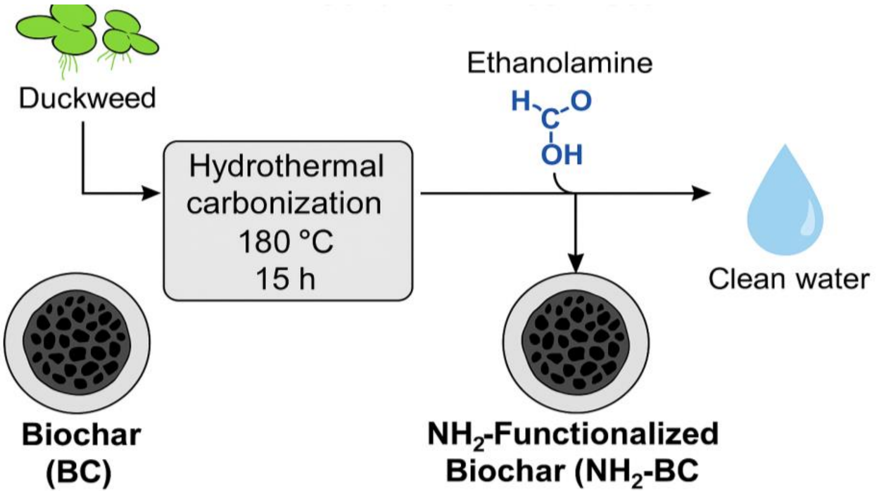
In the pursuit of sustainable and cost-effective materials for environmental remediation, this study reports the facile synthesis of biochar (BC) and amine-functionalized biochar (NH_2-BC) derived from duckweed via hydrothermal carbonization. Duckweed, an abundant aquatic biomass, was subjected to hydrothermal treatment at 180 °C for 15 hours to yield pristine BC. To enhance surface functionality, NH_2-BC was synthesized using ethanolamine as a nitrogen-rich modifier under identical conditions. The straightforward, low-energy synthesis route demonstrates a green and scalable strategy for converting waste biomass into value-added functional materials. These findings position duckweed-derived NH_2-BC as a promising candidate for targeted applications in wastewater treatment, particularly in removing heavy metals and organic contaminants.

Keywords: duckweed-derived biochar; hydrothermal carbonization; amine functionalization; environmental remediation.



Future Chemistry Research Presentation for Undergraduate Students (US-P-021)

Development of silver nanoparticle coated with *Allium sativum* balm stick product for anti-inflammatory in chronic eczema

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Eczema is the most common skin disorder. Current treatments often involve corticosteroids that suppress the immune system and may cause side effects. Garlic, with its anti-inflammatory properties, offers an interesting alternative for treating chronic skin inflammation. In an experiment, active compounds were extracted from fresh garlic using a solvent-free method (crushing and centrifuging) then synthesized into silver nanoparticles form by ionic gelation method. The chemical composition was analyzed using FTIR, GC-MS and SEM techniques, revealing four significant peaks, a compound with anti-inflammatory activity at 0.28% and particle size of approximately 31.28 nm, measured by ImageJ software. The anti-inflammatory and antibacterial effects were tested using albumin denaturation assay and disc diffusion methods. The silver nanoparticles exhibited 95.70% anti-inflammatory efficacy at 25 µg/mL and demonstrated antibacterial activity against *Staphylococcus aureus*, with a clear zone of 0.35 cm. In this experiment, it is expected that a single formula will be used to make the balm, with the ingredients including paraffin wax, 25 µg/mL garlic extract in silver nanoparticles form, vassaline, camphor, menthol, perfume and food coloring. It is suggested that this formulation could be further developed into a prototype balm for combating chronic skin inflammation, with future development plans in place.

Keywords: garlic; silver nanoparticle; anti-inflammatory; antibacterial

Future Chemistry Research Presentation for Undergraduate Students (US-P-022)

Assessing the photocatalytic performance of hydrothermally synthesized Fe-doped $BiVO_4$ under low intensity UV-irradiation

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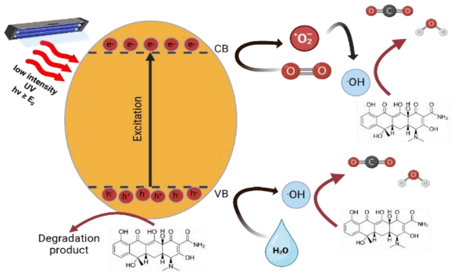
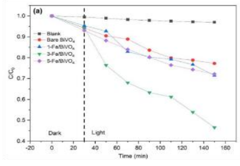
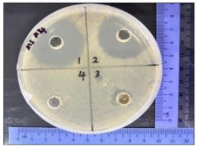
This study demonstrates the potential of Fe-doped $BiVO_4$ as an efficient photocatalyst for the degradation of tetracycline (TC). The Fe-doped $BiVO_4$ was synthesized using the hydrothermal method, resulting in a monoclinic heterostructure with a crystallite size ranging from 27.37 to 29.10 nm, and an optical band gap of 2.69-2.87 eV. Photocatalytic tests revealed that 3 wt% Fe-doping exhibited the highest degradation efficiency, removing 73.37% of TC in 120 minutes under a low-power (13 W) UV lamp. The enhanced photocatalytic performance was attributed to the improved electron-hole separation and optimized Fe doping concentration, which facilitated more efficient light absorption and charge carrier dynamics. Additionally, antibacterial tests confirmed the catalyst's ability to inactivate *Staphylococcus aureus*, even in the absence of light, demonstrating its dual functionality in both pollutant degradation and bacterial inactivation. The cost analysis revealed that the synthesized Fe-doped $BiVO_4$ costs RM 8.17 per gram, further enhancing its appeal for scalable and cost-effective applications. These findings highlight the versatility of Fe-doped $BiVO_4$ as a photocatalyst for addressing antibiotic-based pollution and waterborne pathogens, making it a promising candidate for practical applications in wastewater treatment and environmental remediation. These findings contribute to global efforts in mitigating waterborne antibiotic and microbial pollution, particularly in regions where access to high-energy treatment technologies is limited.

Keywords: bismuth vanadate; hydrothermal; photocatalysis; antibacterial; Fe-doping; environmental remediation





S.aureus inactivation



Future Chemistry Research Presentation for Undergraduate Students (US-P-023)

Synthesis and characterization of zeolite A from fly ash and its applications as potential catalysts for ethanol dehydrogenation process to acetaldehyde

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Catalytic dehydrogenation of ethanol produces acetaldehyde, an important precursor for several value-added chemicals such as acetic acid and acetate esters. In this work, fly ash waste from the BLCP power plant in Rayong Province, Thailand, was utilized as a feedstock to synthesize zeolite A via the hydrothermal method. The study aims to evaluate the catalytic performance of zeolite A derived from fly ash as a heterogeneous catalyst for the dehydrogenation of ethanol to acetaldehyde. The catalysts were characterized using XRD, SEM-EDX, FTIR, and N_2 adsorption-desorption analysis. For the catalytic test, zeolite A from fly ash was used in gas-phase ethanol dehydrogenation at temperatures ranging from 200 to 400 °C. The results revealed that acetaldehyde conversion and selectivity increased as the reaction temperature rose from 200 to 400 °C. Zeolite A from fly ash exhibited high basicity, as measured by CO_2-TPD, resulting in 38% conversion and 34.3% selectivity toward acetaldehyde at 400 °C. The heterogeneous catalyst, zeolite A from fly ash, demonstrates significant potential for the efficient dehydrogenation of ethanol to acetaldehyde.

Keywords: fly ash; zeolite A; dehydrogenation; ethanol; acetaldehyde

High-performance geopolymer from power plant fly ash for heavy metal removal and sustainable waste management

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This study presents the synthesis and application of geopolymer as an adsorbent for Zinc (II) ion removal from aqueous solutions. The geopolymer was prepared using fly ash sourced from the Mae Moh power plant in Lampang Province, activated with 10 M NaOH. Adsorption experiments were conducted to evaluate its efficiency, with a focus on optimizing parameters such as adsorbent dosage and contact time. The results revealed that the optimum conditions were 120 g/L dosage and 60 minutes of contact time, achieving a maximum Zinc (II) removal efficiency of 90.46% at an initial concentration of 25 ppm. The geopolymer exhibited high performance as a low-cost, eco-friendly material, suitable for heavy metal adsorption in wastewater treatment. Furthermore, this approach supports sustainable resource utilization and aligns with the Bio-Circular-Green (BCG) economy model by converting industrial byproducts into value-added materials. The findings highlight the potential of geopolymer as a promising solution for environmental remediation and industrial water treatment.

Keywords: power plant fly ash; geopolymer; adsorption; zinc (II); bio-circular-green (BCG) economy

Nickel oxide/activated carbon (NiO/AC) composite electrodes using nickel sulfate as a precursor for high performance supercapacitors in water in salt electrode (WiSE)

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The development of high-performance supercapacitors is often hindered by low energy and power densities, particularly under elevated voltage conditions. In this study, composite electrodes comprising nickel oxide and activated carbon (NiO/AC) were fabricated using nickel sulfate as a precursor, with the aim of enhancing electrochemical performance in a water-in-salt electrolyte (WiSE) system. NiO was synthesized via a co-precipitation method and characterized using X-ray diffraction (XRD) and scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX). Composite electrodes with varying NiO/AC ratios (1:1, 1:3, and 3:1) were evaluated in a symmetric supercapacitor configuration using a 2.0 V WiSE electrolyte. Electrochemical analyses, including cyclic voltammetry (CV), galvanostatic charge/discharge (GCD), and electrochemical impedance spectroscopy (EIS), revealed that the 1:3 NiO/AC ratio (NC513S) delivered the highest performance, achieving a specific capacitance of 31.23 F/g, energy density of 17.35 Wh/kg, and power density of 208.18 W/kg. The results indicate that the optimized NiO/AC composite, in combination with the extended voltage window of WiSE, offers a promising route for overcoming the limitations of conventional aqueous supercapacitors.

Keywords: nickel oxide (NiO); activated carbon (AC); water-in-salt electrolyte (WiSE)

Future Chemistry Research Presentation for Undergraduate Students (US-P-026)

Effect of NiO calcination temperature on the performance of NiO/AC composite electrodes for symmetric EDLCS in water-in-salt electrolytes

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Nickel oxide (NiO), known for its high theoretical specific capacitance, is a promising material for enhancing electric double-layer capacitors (EDLCs). In this study, NiO was combined with activated carbon (AC) to form composite electrodes aimed at improving conductivity and surface area. The influence of NiO calcination temperature on structural and electrochemical properties was systematically investigated by preparing composites at 400 °C, 500 °C, and 600 °C—denoted as NC513-400 (N400), NC513-500 (N500), and NC513-600 (N600), respectively. A water-in-salt electrolyte (WiSE) based on sodium nitrate ($NaNO_3$) was employed, offering an expanded operating voltage window of up to 2.2 V. Structural analysis via X-ray diffraction (XRD), scanning electron microscopy (SEM), and Brunauer–Emmett–Teller (BET) surface area analysis revealed temperature-dependent variations in crystallinity and porosity. Electrochemical testing demonstrated that the electrode calcined at 500 °C (N500) achieved the best overall performance, showing superior energy and power density as well as enhanced stability. Compared to commercial activated carbon (NC50), the N500 composite displayed notable improvements, making it a strong candidate for high-performance, WiSE-compatible EDLC systems.

Keywords: nickel oxide (NiO); water-in-salt electrolyte (WiSE); electric double-layer capacitors (EDLCs)

Antioxidant activity of root of *Allophylus cobbe* (L.) Raeusch

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This research aims to investigate the antioxidant activity of maceration extracts derived from the roots of *Allophylus cobbe* (L.) Raeusch. Crude extracts were obtained using hexane, dichloromethane, ethyl acetate, and methanol, with the methanol extract yielding the highest amount at 1.61%. Antioxidant activity was assessed using the DPPH radical scavenging assay, where the ethyl acetate extract demonstrated the highest inhibition rate at 95.23% ± 2.00. Further evaluation using the FRAP method revealed an antioxidant capacity of 22.50 ± 0.29 mg of ascorbic acid equivalents per gram of dry extract. These findings provide valuable insights into the antioxidant properties of *Allophylus cobbe* (L.) Raeusch and underscore its potential contribution to medical research and the development of locally sourced medicinal herbs.

Keywords: *Allophylus cobbe* (L.) Raeusch; antioxidant activity; crude extraction; natural products

Future Chemistry Research Presentation for Undergraduate Students (US-P-029)

Green synthesis of silver nanoparticles using leaves extract from *Bambusa beecheyana* Munro and its antibacterial activity

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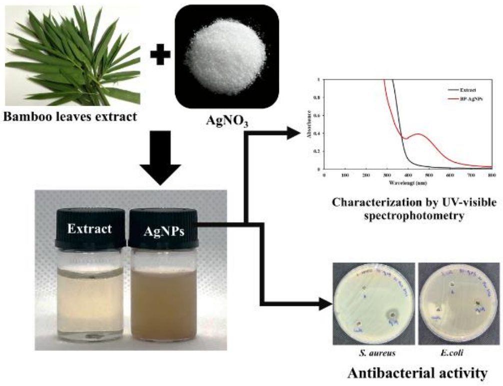
In this study, environmentally friendly silver nanoparticles (AgNPs) were synthesized using herbal extracts derived from the leaves of *Bambusa beecheyana* Munro. The objective was to investigate the synthesis process and evaluate the antibacterial efficacy of the AgNPs against *Staphylococcus aureus* (*S. aureus*) and *Escherichia coli* (*E. coli*). The synthesis was conducted by mixing a 0.5% w/v concentration of *Bambusa beecheyana* Munro leaf extract with 2 mM silver nitrate at 70°C for 15 minutes. The successful formation of AgNPs was indicated by a color change from light yellow to dark brown and further confirmed by UV–visible spectrophotometry, which showed a maximum absorption peak at 442 nm. The antibacterial activity of the synthesized AgNPs was assessed using the agar disc diffusion method, resulting in inhibition zones of 9.33 ± 1.53 mm for *S. aureus* and 8.67 ± 1.15 mm for *E. coli*. These findings demonstrate the potential of agricultural waste, such as *Bambusa beecheyana* Munro leaves, for the green synthesis of AgNPs. Moreover, the synthesized nanoparticles exhibit promising antibacterial properties, paving the way for their application in sustainable antimicrobial development and the value-added utilization of agricultural waste.

Keywords: *Bambusa beecheyana* Munro; silver nanoparticles; antibacterial activity; green synthesis



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Department of Science Service

Driving the Innovation-based Economy Through High-quality and Certified Laboratories

To provide scientific services through regulation, supervision, promotion, research, and development in science and technology, including serving as the national central laboratory for science and technology.

To act as the national accreditation body for promoting and developing the national quality infrastructure system (NQI), particularly in the areas of metrology, testing, calibration, and inspection, to ensure sufficient quality and standards to support the sustainable advancement of the national economy.

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Providing training and skills development for laboratory technical personnel, aimed at enhancing the quality and standards of laboratory operations, including personnel certification in accordance with ISO/IEC 17024.

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An organization designated as a Standard Development Organization (SDO) by the Thai Industrial Standards Institute (TISI) in 15 fields. It provides proficiency testing services for laboratories accredited under ISO/IEC 17043 and offers product certification in accordance with relevant standards.


TISI

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The nation's principal agency for implementing and evaluating physical, biological and chemical testing, accredited under ISO/IEC 17025, including the preparation of reference processes and reference materials. Operations are conducted in accordance with laboratory safety standards, serving as a model for other laboratories nationwide.

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บริษัท พาราไซแอนติฟิค จำกัด เป็นบริษัทชั้นนำของประเทศ ในการนำเข้าและให้บริการแบบครบวงจร สำหรับเครื่องมือวิทยาศาสตร์ และเครื่องมือทดสอบด้านวิศวกรรม จากผู้ผลิตชั้นนำที่มีชื่อเสียงของโลก โดยเฉพาะอย่างยิ่งบริษัทฯ ได้เป็นตัวแทนจำหน่ายแต่เพียงผู้เดียวในประเทศไทย สำหรับเครื่องมือวิทยาศาสตร์ และเครื่องทดสอบของ **Shimadzu** ซึ่งเป็นบริษัทชั้นนำของประเทศญี่ปุ่น มานานกว่า 30 ปี

เพื่อให้ลูกค้าของบริษัทฯได้รับความพึงพอใจสูงสุด บริษัทฯได้มีการพัฒนาประสิทธิภาพในการให้บริการแก่ลูกค้า โดยได้มีการนำระบบ **คุณภาพมาตรฐาน ISO 9001:2015** มาใช้ในการบริหารงาน และบริษัทฯ ยังสามารถให้ **บริการสอบเทียบเครื่องมือตามมาตรฐาน ISO/IEC 17025:2005** สำหรับเครื่อง UV-VIS Spectrophotometer และเครื่อง Universal Testing Machine และจะขยายขอบเขตเพื่อให้ ครอบคลุมการสอบเทียบเครื่องมือชนิดอื่นๆต่อไป

และการที่ บริษัท พาราไซแอนติฟิค จำกัด เป็นบริษัทใน **กลุ่มบริษัท พาราวินเซอร์ จำกัด** ซึ่งเป็นองค์กรขนาดใหญ่ชั้นนำของประเทศ ทำให้บริษัทฯ มีศักยภาพสูง สามารถให้บริการลูกค้าได้ทุกระดับ ซึ่งรวมถึงการจัดซื้อ ที่เป็นโครงการขนาดใหญ่

สำหรับลูกค้าของบริษัทฯ ได้ครอบคลุมทั้งกลุ่มลูกค้าราชการและเอกชน เช่น

- มหาวิทยาลัยและสถาบันการศึกษาต่างๆ
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- สถาบันค้นคว้าวิจัยด้านวิทยาศาสตร์
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- LC-MS/MS (Triple Quadrupole)
- LCMS-Q-TOF MS
- LCMS-IT-TOF MS
- LC-MS (Single Quadrupole)
- GC-MS/MS
- GC-MS

Life Science Research
- Imaging Mass Microscope
- MALDI TOF(/TOF) Mass Spectrometer
- Microorganism Identification (MALDI TOFMS)
- Microchip Electrophoresis (DNA/RNA Analysis)
- Functional Near-infrared Spectroscopy System for Research

Physical Properties Analyser
- Thermal Analyzer
- Particle Size Analyzer
- Total Organic Carbon Analyzer

Scientific Equipment

Elemental Analyzer Group
- Energy Dispersive X-Ray Fluorescence Spectrometer
- Optical Emission Spectrometer

Surface Analyzer Group
- Scanning Probe Microscope
- Electron Probe Micro Analyzer
- X-Ray Photoelectron Spectroscopy

Testing Machine
- Universal Testing Machines
- Fatigue Tester Machine
- Hardness Tester
- Viscosity Testers
- Special Purpose Tester

Non-Destructive Testing
- Microfocus X-ray System
- Microfocus X-ray CT System
- Dimensional X-ray CT System

Informatics
- LabSolutions CS
- LabSolutions Bix
- Caliber LIMs

GL Sciences Inc.		**GC & HPLC Accessories** GC & HPLC Column & Accessories Equipment for VOCs & Positive List
DAICEL		**CHIRALPAK® CHIRALCEL® CROWNPAK®** Chiral Stationary Phase
Shodex		**Shodex HPLC Column** Sugar Analysis Column GPC Column
MBRAUN		**Inertgas Technology** Glove Box System Solvent Purification System
KUBOTA		**Centrifuges** Table-top Centrifuge High Speed Refrigerated Centrifuge
EYELA		**Laboratory Equipment** Rotary Evaporators Low Temperature Circulator
TOKI SANGYO		**Viscosity Measurement** Portable Viscometer Digital Viscometer
TAITEC		**Shaker Technology** Incubator Shaker Water Bath
NMReady		**Desk Top NMR** NMReady-60MHz : 1H, 7Li, 13B, 13C, 19F, 31P NMReady-100MHz : 1H, , 13C, 19F, 31P
AS ONE		**AS ONE** General Lab Equipment Consumable & Supplies
Biotage		**Sample Preparations, Purification and Chemical Synthesis** Automated Sample Preparation Instruments Flash Purification Chromatography
IES		**Isolate Extraction Systems Inc.** Supercritical Fluid CO2 Extraction Commercial Series (10, 20, 40 L)
Greatwall		**Greatwall** Glass Reactor Rotary Evaporator

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Advances in Nutraceutical Chemistry Shaping the Future of Disease Prevention in Asia

Dr. Natphasuth Patthirasinsiri

The Role of Natural and Organic Ingredients as Emerging Nutrition Trends

Dr. Kampol Poophawattanakij

Buying Health on the Shelf : New life-changing healthy products in stores 2025

Mr. Jakraphan Punyapapha

Branding plays an important role in consumer products market, anyhow, in Health Products Market, there's still some room to improve.

Mr. Nguyen Deinj Trung

Nutraceutical Market in Practice in Vietnam Presented by: Ted Nguyen, CEO of GT Innovation

Pharmacist.Yodchai Tangjaideborisut

Nutraceutical Market in Practice in Vietnam Presented by: Ted Nguyen, CEO of GT Innovation

Dr. Karsidete Teeranitayatarn

A Functional Nutraceutical for Appetite Stimulation and Gut Health in Companion Animals- MEWLICIOUS

Dr. Uracha Ruktanonchai

Nano-Enhanced Nutraceuticals: Pioneering Solutions for Next-Generation Preventive Healthcare

Assoc. Prof. Dr. Supakorn Boonyuen

Microwave-Assisted Biosynthesis of Quercetin-Stabilized Gold Nanoparticles with Enhanced Antibacterial and Catalytic Properties

Asst. Prof. Pariya Na Nakorn

Anthocyanin Rich-Berry extracts coated magnetic Fe_3O_4 bionanocomposites and their antibacterial activity

Dr. Paramasivam Shanmugam

Green synthesis of silver and gold nanoparticles using Oroxylum indicum plant extract for catalytic and antimicrobial activity

การให้บริการแสงซินโครตรอน

สถาบันวิจัยแสงซินโครตรอน (องค์การมหาชน)
Synchrotron Light Research Institute (Public Organization)

สำหรับภาครัฐและการศึกษา

เทคนิคแสงซินโครตรอนที่ให้บริการแยกตามกลุ่มงานวิจัย

กลุ่มงานวิจัย	เทคนิค
วัสดุศาสตร์และวิศวกรรมศาสตร์ (Materials Science and Engineering)	XTM PES/PEEM/XPS XAS SAXS DXL/MES XRD Residual stress
วิทยาศาสตร์พื้นผิวและฟิล์มบาง (Surface, Interface and Thin films)	PES/PEEM/XPS XRR GIXRD GIXAS
พอลิเมอร์ (Polymers)	XTM SAXS IR
ฟิสิกส์ (Physics)	XTM XAS DXL/MES XRD
วิทยาศาสตร์ชีวภาพและวิทยาศาสตร์สิ่งมีชีวิต (Biological and Life Science)	XTM XAS IR SAXS DXL/MES Micro-XRF TXRF XRF
อาหารและเกษตร (Food and Agricultural Science)	XTM XAS IR SAXS Micro-XRF TXRF XRF
วิทยาศาสตร์พื้นพิภพธรณีวิทยาและโบราณคดี (Earth Science, Gemology and Archaeology)	XTM XAS XRD Micro-XRF TXRF XRF
วิทยาศาสตร์สิ่งแวดล้อม (Environmental Science/ Food and Agricultural)	XTM PES/PEEM/XPS XAS IR SAXS
ไมโครและนาโนเทคโนโลยี (Micro and Nanotechnology)	DXL/MES SAXS micro-XRF

เทคนิคแสงซินโครตรอนที่ให้บริการ

1 X-ray Absorption Spectroscopy (XAS,TR-XAS,GIXAS)

2 X-ray Fluorescence Spectroscopy and Imaging (XRF,TXRF, Micro-XRF)

3 X-ray Diffraction (PXRD, GIRXD)

4 Macromolecular Crystallography (MX,XRF,XAS)

5 Small and Wide-angle X-ray Scattering (SWAXS)

6 X-ray Tomographic Microscopy (XTM)

7 Photoelectron Emission Spectroscopy (PES,XPS,NEXAFS,UPS,VUV)

8 Photoemission Electron Microscopy (PEEM)

9 Infrared Spectroscopy and Imaging (IR)

10 Deep X-ray Lithography (DXL,MES)

สำหรับภาคเอกชน

กลุ่มอุตสาหกรรมเป้าหมาย

1 อุตสาหกรรมอาหารและการเกษตร

2 อุตสาหกรรมวัสดุขั้นสูง

3 อุตสาหกรรมยา สมุนไพร และเครื่องสำอาง

4 อุตสาหกรรมพลังงาน

5 อุตสาหกรรมอัญมณี

ประเภทการให้บริการ

1 บริการเทคนิคแสงซินโครตรอน (Synchrotron Light Service)	4 บริการเทคนิคและวิศวกรรม (Technical & Engineering Service)
2 บริการที่ปรึกษา (Consultancy Service)	5 บริการเครื่องมือวิทยาศาสตร์พื้นฐาน (Scientific Instrument Service)
3 บริการวิจัยตอบโจทย์ (Total Solutions Service)	6 บริการถ่ายทอดเทคโนโลยี (Tech Transfer Service)

กลุ่มเครื่องมือวิเคราะห์ทดสอบ

- Dispersive Raman Microscope
- FT-Raman Spectrometer
- SENTERRA II with FT-RAMAN module
- Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS)
- FTIR Micro-Spectrometer
- UV-Vis spectrophotometer
- X-ray Diffractometer (XRD)
- Wavelength dispersive X-ray Fluorescence (WD-XRF
- Gas Chromatography – Mass Spectrometry (GC-MS/MS)
- Gel Permeation Chromatography (GPC)
- Ultra-High Performance Liquid Chromatography (UHPLC)
- High-Resolution Mass Spectrometry (LC-HRMS)

กายภาพ (งานจุลทรรศน์)

- Atomic Force Microscope (AFM)
- Scanning electron microscope (SEM)
- Transmission electron microscope (TEM)
- X-ray Photoelectron spectroscopy (XPS)

ขั้นตอนการใช้บริการแสงซินโครตรอนสำหรับภาครัฐและภาคการศึกษา

1 ประกาศรับข้อเสนอโครงการ

2 ยื่นข้อเสนอโครงการเพื่อขอใช้บริการแสงฯ ผ่านระบบ Beamline Application System https://user.slri.or.th

3 คณะกรรมการประเมินข้อเสนอโครงการ

4 จัดสรรเวลาการเข้าใช้บริการแสงซินโครตรอน และแจ้งเวลาการเข้าใช้บริการฯ ไปยังผู้ขอใช้บริการ

5 ผู้ขอใช้บริการแจ้งยืนยันการเข้าใช้บริการ

6 อบรมความปลอดภัยผ่านระบบออนไลน์ https://straining.slri.or.th/home

7 รับอุปกรณ์และเข้าทำการทดลอง

8 คืนอุปกรณ์และรายงานผลการทดลองผ่านระบบ Beamline Application System https://user.slri.or.th

ขั้นตอนการขอรับบริการสำหรับภาคเอกชน

1 ยื่นแบบฟอร์มขอรับบริการได้ที่ https://bdd.slri.or.th/bdd

www.slri.or.th/bdd

2 ประเมินและเสนอราคา

3 ตรวจสอบใบเสนอราคาและออกใบสั่งซื้อ / สั่งจ้าง

4 เริ่มให้บริการวิจัย/วิเคราะห์/ผลิตชิ้นงาน

5 ชำระค่าบริการวิจัย/วิเคราะห์/ผลิตชิ้นงาน

6 รายงานผลการวิเคราะห์/วิจัย/ส่งมอบงาน

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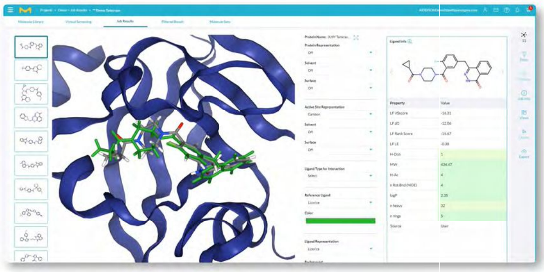

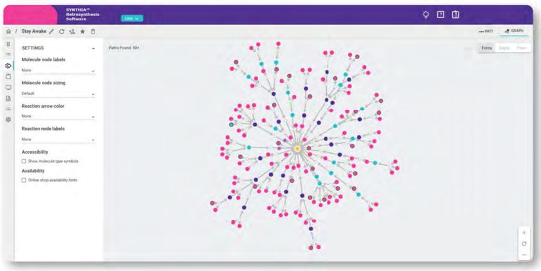

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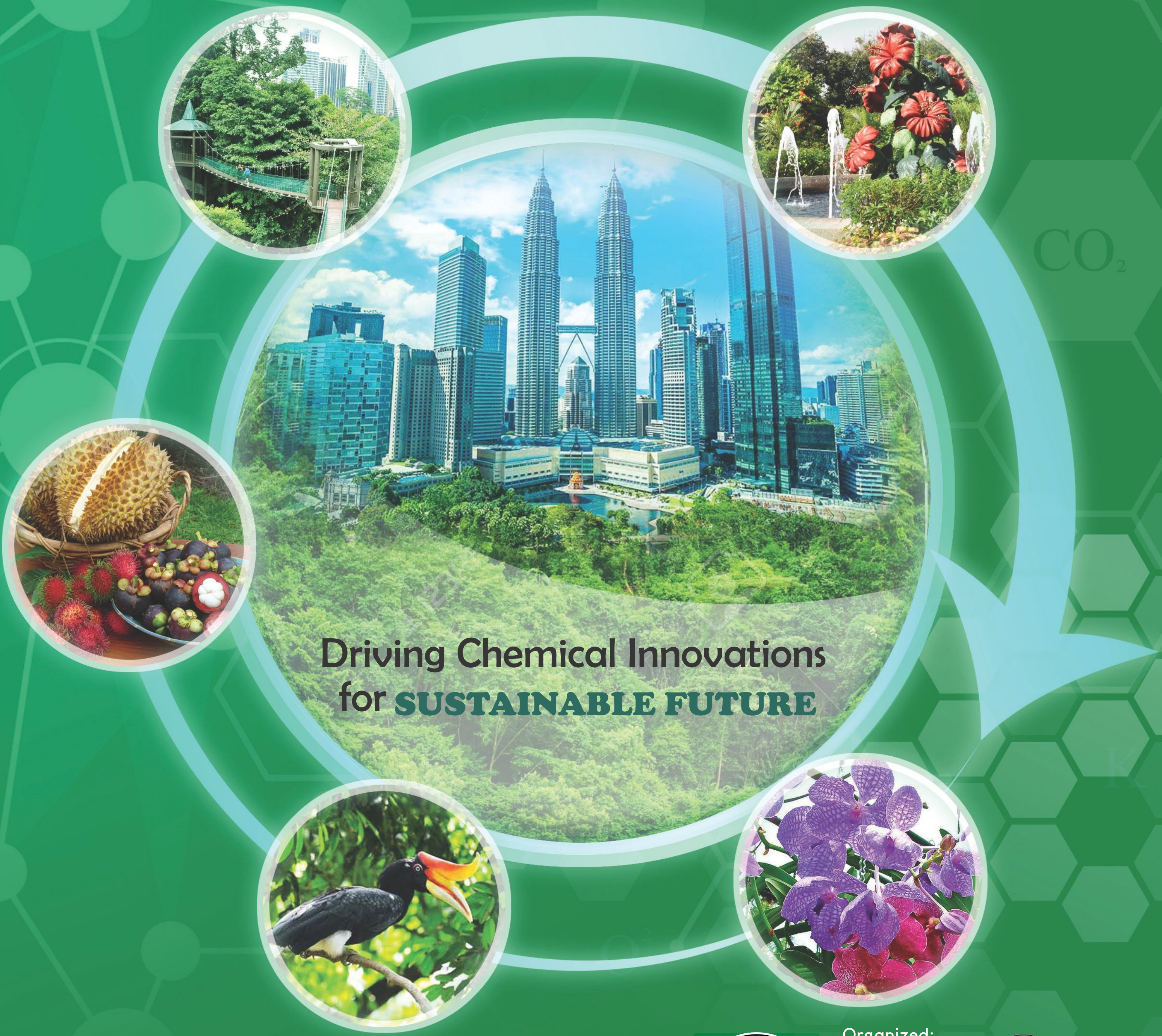

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Chemical Societies (FACS)

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Institut Kimia Malaysia (IKM) is a professional scientific organisation with strong support from our members, the government, the chemical industry, academia, and the corporate and service sectors. With decades of experience and expertise, IKM is proud to host the 21st Asian Chemical Congress (21ACC) and the 23rd General Assembly of FACS (23GA-FACS) in 2027. This prestigious event also marks a significant milestone — the celebration of IKM's 60th anniversary.

Malaysia – truly Asia

Malaysia is a captivating tourist destination that truly reflects the richness of Asian culture, values, arts, architecture, and a wide variety of culinary delights. We are also proud of our million-year-old tropical rainforests, home to one of the world's largest varieties of flora and fauna. Malaysians are well known for their warm hospitality, making every visitor feel genuinely welcome.

KUALA LUMPUR , MALAYSIA

-THE PERFECT PLACE TO MEET

Safety, Stability and Security

Malaysia is a safe, stable, and secure country. As a multiracial and multicultural society, people of various races, ethnic groups, cultures, and beliefs live together in peace and harmony. Malaysia was ranked the 18th safest and most peaceful country out of 163 nations in the Global Peace Index 2022 — a testament to its social stability and welcoming environment.

Strategic Location and Ease of Accessibility

Malaysia is strategically located in the heart of Southeast Asia, with Kuala Lumpur easily accessible from around the globe. More than 60 international airlines fly directly to Malaysia, connecting 135 major cities across 35 countries — including Australia, the UK, and the USA. This makes Malaysia a convenient and well-connected destination for travellers worldwide.

Transportation and Connectivity

Kuala Lumpur is well-connected by major international airlines, while transportation within Malaysia is supported by an extensive network of roads and railways. In the city, a variety of transport options are available — including taxis, ride-hailing services, buses, and mass rapid transit — all at affordable and reasonable prices, ensuring convenient and efficient travel for visitors.

Value for Money and Shopping

Malaysia offers excellent value for money across accommodation, shopping, transportation, internet, and telecommunication services. It is also a renowned food haven, with a wide variety of cuisines — from Chinese, Cantonese, and Indian to Japanese, Korean, Western (including Italian and French), as well as rich and diverse local Malay dishes — all at affordable prices.

English as a medium of communication in Malaysia

In addition to Malay as the national language, Chinese and English are widely spoken throughout Malaysia. English is commonly used as a medium of instruction in education, including universities and research. It is also the primary language in telecommunications, the internet, business, and trade, making communication seamless for international visitors and professionals.

Top-Class Convention Facilities

Malaysia boasts some of the best convention and exhibition infrastructure in the world. Accommodation options range from economical to luxury, catering to all needs and budgets. As a preferred destination for meetings and conferences, the Kuala Lumpur Convention Centre (KLCC) offers state-of-the-art facilities, including 33,659 sqm of space with a capacity for 3,000 attendees. The venue features a plenary hall, conference halls, ballrooms, and a plenary theatre — making it an ideal choice for large-scale events.

21ACC – A THEMATIC SESSION ON CHEMISTRY

- **Theme 1: Chemistry for Sustainability**
- **Theme 2: Chemistry for Energy and Resources**
- **Theme 3: Chemistry for the Environment and Climate Change**
- **Theme 4: Chemistry and Society**
- **Theme 5: Chemistry Education**
- **Theme 6: Young Scientists Programme**

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