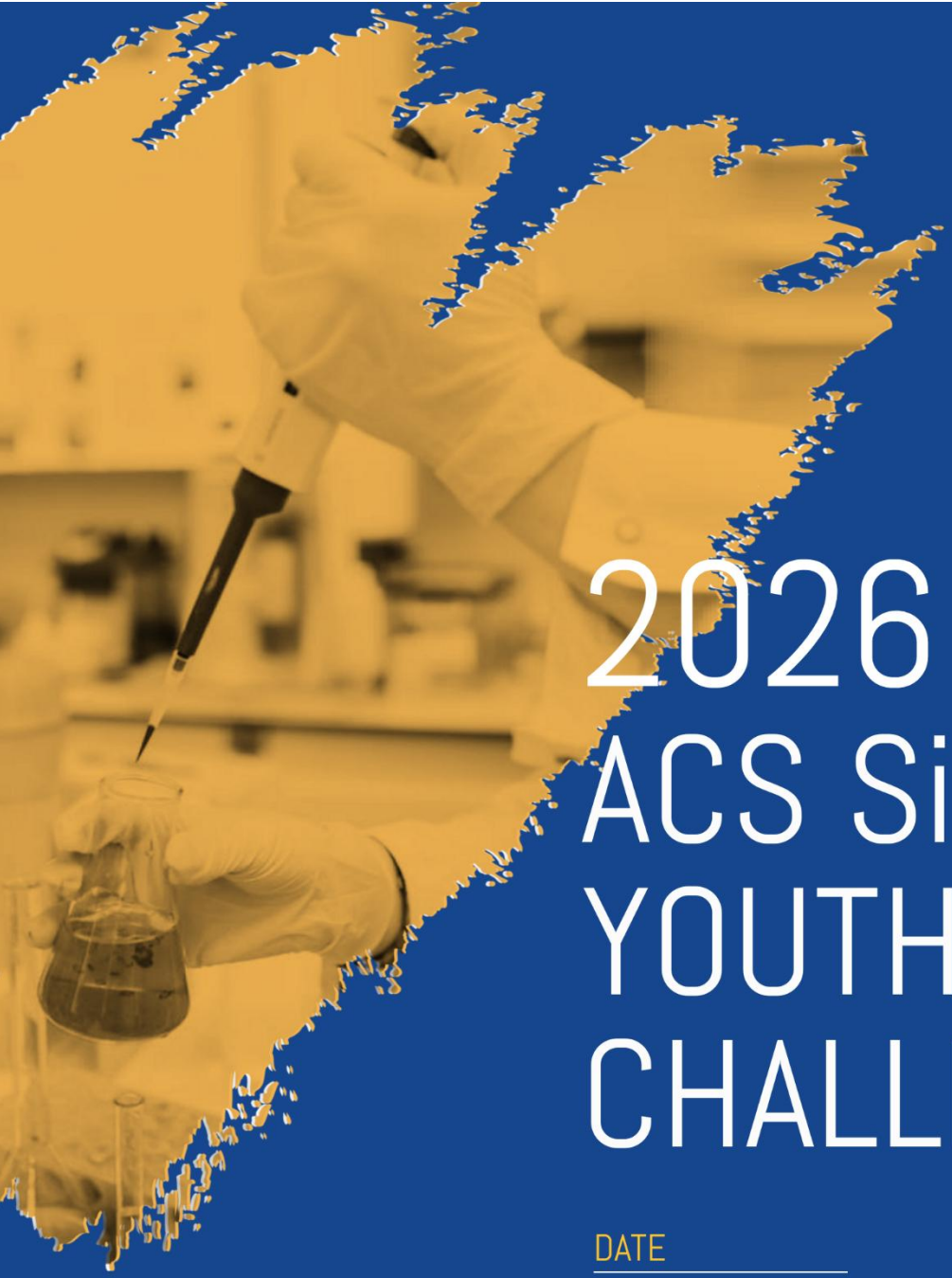

ACS Chapter Singapore

CELEBRATING ACS150 Chemistry is Everything

2026 ACS Singapore YOUTH CHALLENGE

DATE

14 February
9 am – 5 pm

VENUE

Wee Cho Yaw Plaza
Nanyang Technological University
639956, Singapore

Book of Abstracts

TARGET AUDIENCE

Pre-university

University

Chemical Sciences Professionals

American Chemical Society Singapore Youth Challenge 2026

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Dr. Rui A. Gonçalves, Co-Chair
Dr. Rochelle Silva, Co-Chair
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14 February 2026

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9:15am – 9:45am	**Pat GUIRY,** University College Dublin, Ireland *Why is asymmetric synthesis so important?*
9:45am – 10:00am	**Group Photo**
10:00am – 11:30am	**AM session** (Wee Cho Yaw Plaza – Auditorium, Level 1) Chair: Brendan Burkett, A*STAR, Singapore
10:00am – 10:30am	**J. Justin GOODING,** The University of New South Wales, Australia *Science fiction becoming science fact for diagnosing and treating cancer*
10:30am – 11:00am	**Yeng Ming LAM,** Nanyang Technological University, Singapore *Can polymers ever be sustainable?*
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2:00pm – 2:30pm	**Fun Man FUNG,** University College Dublin, Ireland *Chemistry is everything, but what can you see?*
2:30pm – 3:00pm	**Feng LI,** Sichuan University, China *Chemical tools for ultrasensitive detection of gene mutations*
3:00pm – 3:30pm	**Closing Ceremony & Prizes**
3:30pm – 4:00pm	**Coffee Break**
4:00pm – 5:00pm	**ACS Singapore Chapter Annual General Meeting**

(updated as of 12 Feb 2026)

Abstracts of Oral Presentations

Why is asymmetric synthesis so important?

Pat Guiry[1]

[1]*School of Chemistry, University College Dublin, Ireland*

The preparation of enantiomerically pure compounds is an important area of research in modern organic chemistry. Asymmetric synthesis is technologically employed to prepare just one hand of a pair of enantiomers and of the possible approaches, asymmetric catalysis offers the most potential in terms of atom efficiency and environmental considerations. The asymmetry of a metal-catalysed process is controlled by the organic groups (ligands) bound to the metal as they control the binding of reactants and their reaction paths through steric and electronic interactions. Particular metals catalyse specific transformations of interest to synthetic chemists involved in medicinal chemistry and materials chemistry research programmes in academia and industry. This lecture will give the background to the importance of this research topic and will include some recent results from our research group on developing Pd-catalysed decarboxylative transformations, and the development of novel planar chiral cyclophane-containing ligands and their application in [3+2] cycloadditions.

Science fiction becoming science fact for diagnosing and treating cancer

J. Justin Gooding[1*]

[1]*The School of Chemistry and Australian Centre for NanoMedicine, The University of New South Wales, Australia*

**E-mail:* Justin.gooding@unsw.edu.au

This multimedia presentation will focus on the inspiration that science fiction films such as *The Fantastic Voyage*, *Gattaca*, and *Frankenstein* have given research scientists in general and researchers at the Australian Centre for NanoMedicine in particular. The talk will show how the ideas from these old movies with regards to diagnosing and treating human diseases, which might have been dreams at the time, have progressed to reality today. The talk will cover developments in biosensors, drug delivery and even the 3D bioprinting of model cancers. The importance of these developments to improving human health will be discussed. The presentation is suitable for anybody with an interest in science or an interest in movies.

Can polymers ever be sustainable?

Yeng Ming Lam[1, 2]
[1]*School of Materials Science and Engineering, Nanyang Technological University, Singapore*
[2]*Facility of Analysis, Characterization, Testing and Simulations, Singapore*

The global production of polymers has exceeded 9 billion tons, driven by their extensive applications in areas such as packaging, biomedical, and electronic devices. Traditional polymers, including polyethylene, polypropylene, polyethylene terephthalate (PET), polyvinyl chloride (PVC), and nylon, are predominantly synthesized from petrochemical sources. These materials present significant environmental challenges, particularly due to their energy-intensive production processes and complex recycling protocols. Consequently, substantial quantities of these polymers ended up in landfills or if the waste collection channels are less well developed, eventually contribute to environmental pollution.

Given the formidable challenge of completely replacing these traditional polymers with sustainable alternatives, a pragmatic approach is to enhance recycling and upcycling strategies. This presentation will discuss on how in-depth understanding for degradation processes can lead to more effective methodologies for the recycling of one engineering plastics - polyamides. Different strategies are required for the recycling of different polymers, in this talk I will also cover the enzymatic degradation of PET, focusing on how the polymer's physicochemical properties influence the design of platforms for high-throughput enzyme library screening, aimed at improving degradation efficiency. The discussion will include the effects of substrate crystallinity and microstructure on the degradation kinetics of PET and its copolymers, such as poly(ethylene terephthalate-co-isophthalate) and poly(ethylene terephthalate-co-butylene terephthalate), as well as branched PET variants.

Parallel to these efforts, the development of biodegradable polymers and biopolymers derived from renewable resources, such as cellulose, starch, proteins, lignin, and chitin, represents a promising avenue. These materials not only have a reduced carbon footprint but also offer biodegradability under appropriate conditions. The presentation will also cover advances in the application of cellulose-based materials in agriculture and biomedical, emphasizing their potential as sustainable alternatives. This talk will attempt to provide a comprehensive overview of different approaches to mitigate the environmental impact of synthetic polymers through advanced recycling technologies and the development of sustainable polymeric materials.

From active-site dyads to substrate scope: mechanistic insights into f_{420}-dependent dehydrogenases

Kayunta Johnson-Winters[1]

[1]*Department of Chemistry and Biochemistry, The University of Texas at Arlington, United States*

F_{420}-dependent dehydrogenases play central roles in microbial redox metabolism, yet the catalytic principles governing substrate specificity, hydride transfer, and product formation across this enzyme family remain undefined. Here, we combine detailed mechanistic studies of *Mycobacterium tuberculosis* (*Mtb*) F_{420}-dependent glucose-6-phosphate dehydrogenase (FGD) with kinetic and functional characterization of newly identified F_{420}-dependent sugar-6-phosphate dehydrogenases (FSDs) from *Cryptosporangium arvum* and Nocardia to elucidate conserved and divergent features of F_{420}-dependent catalysis.

Using thermodynamic, steady-state, and pre steady-state kinetic analyses of *Mtb*-FGD variants, we identify a previously unrecognized catalytic dyad composed of H40 and E13. Temperature-dependent pH profiles and diethylpyrocarbonate inactivation experiments establish H40 as the active-site base responsible for proton abstraction from glucose-6-phosphate, while E13 functions in proton relay, enabling efficient hydride transfer to the C5 position of F_{420}. Global kinetic analysis further reveals rapid chemistry followed by slower product release, with cofactor association contributing to rate limitation.

In parallel, characterization of *C. arvum* and Nocardia FSDs reveals broadened substrate scope and unexpected functional complexity. While glucose-6-phosphate remains the preferred substrate, fructose-6-phosphate and mannose-6-phosphate are also oxidized. NMR and mass spectrometry demonstrate that fructose-6-phosphate undergoes isomerization to glucose-6-phosphate prior to oxidation, revealing dual isomerase–dehydrogenase activity. Despite substrate diversity, hydride transfer is not rate-limiting, and no catalytic intermediates accumulate.

Together, these studies define key catalytic determinants governing F_{420}-dependent redox chemistry and uncover functional versatility within this enzyme family, providing a framework for understanding F_{420} enzyme evolution and informing future therapeutic targeting strategies.

Chemistry is everything, but what can you see?

Fun Man Fung[1]

[1]*School of Chemistry, University College Dublin, Ireland*

Learning chemistry requires bridging the gap between the macroscopic world we observe and the abstract, particulate universe that governs it. While chemistry constitutes "everything" around us, students often ask: W*hat can I see?* Novice learners struggle to visualize dynamic molecular mechanisms, resulting in high cognitive load, anxiety, and a reliance on rote memorization. To address this visualization gap, we present a decade of research on Technology-Enabled Blended Learning Experience (TEBLE) that renders the inaccessible visible through a synergistic Human-Computer Interaction (HCI) framework.

Chemical tools for ultrasensitive detection of gene mutations

Feng Li[1*]

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Rare nucleic acid mutations, such as single nucleotide variants (SNVs), are essential biomarkers for precision medicine, with important clinical applications ranging from cancer to prenatal diagnosis and to infectious diseases. Sensitive profiling of SNVs with low variant-allele frequencies (VAFs) in the presence of high concentrations of wild-type (WT) sequences is crucial for the detection of cancer mutations in cell-free DNA (cfDNA) or fetal mutations in maternal plasma. Over the past years, research in our laboratory focuses on the rational design of DNA hybridization probes capable of detecting rare nucleic acid mutations in clinical samples with single nucleotide precision. By digging into the thermodynamics of nucleic acid hybridization reactions, we have developed a set of tools that enable the accurate measurement and control of key thermodynamic parameters of hybridization probes for discriminating single nucleotide mutations. Moreover, we have also introduced new reactions and reaction networks, allowing the robust discrimination of mutations at wide temperature and concentration ranges, which were further translated into improve clinical outcomes for cancer liquid biopsy. In this presentation, I will give a comprehensive overview of our effort for the rational design and clinical applications of such hybridization probes.

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List of Poster Presentations

Reference Number	Abstract Title	Presenters
YC26-0010	Valence State-Dependent Catalytic Behavior of Ni and Co in NiCo/Activated Carbon Derived from Spent Li-ion Batteries for Biojet Fuel Production	Adyatma Bhagaskara
YC26-0020	From Atoms to Armor: Development of a next-generation multilayered flexible nanocomposite for radiation shielding	Adviteeya Krishna, Logan Wong Duran
YC26-0030	Zinc Single-Atom Nanozyme as Carbonic Anhydrase Mimic for CO2 Capture and Conversion	Eslam M. Hamed
YC26-0040	Precisely Manipulating Polymer-Chain-Interactions for Multifunctional Hydrogel	Shuai Guo
YC26-0050	Benchmarking foundation potentials against quantum chemistry methods for predicting molecular redox potentials	Yicheng Chen
YC26-0060	Formulation of water-based barrier coatings for sustainable packaging	Guan Ji, Lim
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YC26-0080	Enhancement of Ultraviolet Resistance of Polyaspartics Using Metal Oxide Particles	Bahar Demirtaş Karabacak
YC26-0090	Optimization of hydrogel sunscreen systems containing Phenylbenzimidazole Sulfonic Acid, Terephthalylidene Dicamphor Sulfonic Acid, and Disodium Phenyl Dibenzimidazole Tetrasulfonate for transparency, stability, and sensory performance	Teng Yih Lee
YC26-0100	Reversible anti-fouling coating for sustainable and reusable reverse osmosis membranes	Renee Yong
YC26-0110	Uncertainty-aware active learning for screening lead-free halide perovskites	Xiyao Yu
YC26-0120	A Hybrid Physics-Driven Neural Network Force Field for Liquid Electrolytes	Junmin Chen
YC26-0130	Selective electrochemical oxidation of primary alcohols to aldehydes in organic electrolytes	Hui Wen Neo
YC26-0140	Edge Functionalisation of Curved Nanographenes	Mahalakshmi Anand
YC26-0150	Forced degradation of a block copolymer to guide stability considerations in polymeric nanoparticle formulation development	Mervin Woon Jie En
YC26-0160	Motif-driven scalable design of rutile high-entropy oxide catalysts for oxygen evolution reaction	Guanpeng Ren
YC26-0170	Investigating the use of a hybrid Fmoc-D-Phe-alginate hydrogel as a drug delivery medium for wound-related pain treatment	Michiko Shen
YC26-0180	Shear-aligned bioprinting of chitosan hydrogels for programmable, multidirectional actuation	Chloee Jing Yu Chong
YC26-0190	Controlling evaporation driven growth of single crystals as a model for chiral materials	Kendrick Lius Bong
YC26-0200	Chitosan-Induced Rapid and Controllable Hydrogel Degradation for Biomedical Uses	Kayden Qirong Liu

YC26-0210	Aldehyde quantification using novel fluorometric assay of Galactose Oxidase activity	Chong Yik Lim
YC26-0220	Synthesis of Extended Nanographenes	Saroj Ali
YC26-0230	Controls on trace metal accumulation in mangrove sediments of Singapore: Implications for coastal ecosystem management	Crescentia Aw Lee Hong
YC26-0240	Bio-based microgels as a sustainable delivery system for phosphate fertilizers	Ervin Booi
YC26-0250	Profiling of nutraceuticals in stingless bee propolis extract using UV spectroscopy and GC-MS	Kaelyn Pon
YC26-0260	Tunable Ru PNP catalysts for the hydrogenation of carbon dioxide to methanol	Kai Bin Jonathan Chan
YC26-0270	Chemical fate of carbon and nutrients during sustainable microalgal growth in palm oil mill effluent.	W.M.S. Dayanath
YC26-0280	Discovery of bioactive peptidoglycan fragments from Lactobacillaceae that confer intestinal protection in hosts	Yaquan Liang
YC26-0290	Polymerizable Deep Eutectic Solvents for Simultaneous Cellulose Nanofibrillation and In-Situ Polymerization	Udyani Aloka Weerasinghe
YC26-0300	Fully Cyclized Corannulene-Based Curved Nanographenes: Structural Elucidation and Optimized Synthesis	Jian-Wen Wong
YC26-0310	Machine learning-based SERS chemical space for two-way prediction of structures and spectra of untrained molecules	Jaslyn Ru Ting Chen
YC26-0320	Engineering Waste-Derived Silicate Activators for High-Performance and Scalable Geopolymer Concrete	G.G.T.D. Wickramathilake
YC26-0330	Chemistry-informed e-waste recycling operations for informal recyclers targeting critical metals in the net-zero pathway	Pasindu Arunapriya
YC26-0340	Valorization of okara and okara-derived substrates through Pleurotus ostreatus mycelium biotransformation	Malsha Samarasiri

Abstracts of Poster Presentations

Catalytic Role of Ni and Co Valence States in NiCo/Activated Carbon Derived from Spent Li-ion Batteries for Biojet Fuel Production

Adyatma Bhagaskara[1], Wega Trisunaryanti[1*], Karna Wijaya[1], Dita Adi Saputra[2]
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[2]*Research Center for Conversion and Energy Conservation, National Research and Innovation Agency (BRIN), The B.J. Habibie Science and Technology Area, South Tangerang, Banten 15314, Indonesia.*
[*]*E-mail: wegats@ugm.ac.id*

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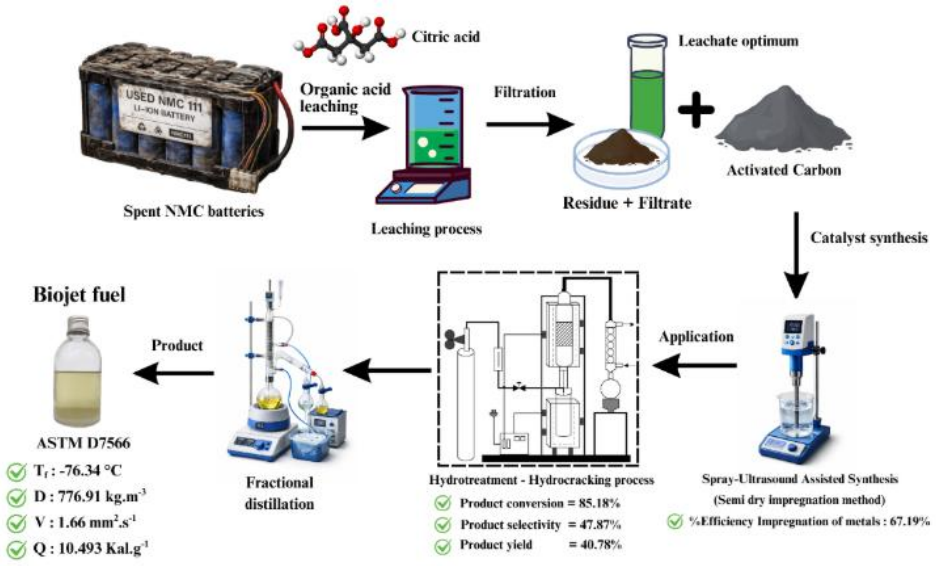
The increasing demand for sustainable energy and waste valorization has driven efforts to convert spent lithium-ion batteries (LIBs) and renewable biofeedstocks into value-added products. This study investigates the effect of nickel and cobalt valence states recovered from spent nickel–manganese–cobalt (NMC) cathodes on the bifunctional catalytic performance of NiCo supported on activated carbon (NiCo/AC) for palm oil hydrotreatment to biojet fuel. Citric acid–based leaching without a reducing agent enables efficient recovery of Ni and Co, achieving leaching efficiencies of 84.95% and 86.90%, while sonication-assisted synthesis can improves metal impregnation efficiency. X-ray photoelectron spectroscopy (XPS) and ammonia temperature-programmed desorption (NH_3-TPD) analyses reveal that mixed oxidation states (Ni^0/Ni^{2+} and $Co^0/Co^{2+}/Co^{3+}$) generate synergistic hydrogenation–acidic sites, enhancing selectivity toward C_8–C_{16} hydrocarbons. Catalytic tests show that NiCo/AC achieves 85.18% conversion, 47.87% selectivity, and a biojet fuel yield of 40.78% at 350 °C. The resulting biojet fuel satisfies ASTM D7566 specifications, exhibiting a freezing point of –76.34 °C, density of 776.91 kg m^{-3}, kinematic viscosity of 1.66 mm^2 s^{-1}, and heating value of 10.493 kcal g^{-1}, confirming its suitability for sustainable aviation fuel applications.

Keywords: biojet fuel; hydrotreatment process; NiCo/AC; Spent NMC cathode; valence state



From Atoms to Armor: Development of a next-generation multilayered flexible nanocomposite for radiation shielding

Adviteeya Krishna[1*], Logan Wong Duran[1*]
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Ionizing radiation, including gamma photons and neutrons, presents serious hazards across sectors such as nuclear energy, aerospace and medical diagnostics. Traditional shielding materials like lead provide high attenuation but suffer drawbacks including toxicity, rigidity and environmental concerns. These limitations highlight the need for flexible and sustainable materials that can effectively protect against multiple radiation types.

In this study, we developed a multilayered polymer nanocomposite. Four radiation-functional nanofillers were integrated within different layers of a matrix to exploit complementary interaction mechanisms. Bismuth nanoparticles were selected for strong interaction with gamma photons, gadolinium oxide nanoparticles were incorporated for their high thermal neutron absorption cross-section, zirconium oxide was included to provide mechanical reinforcement and chemical stability, and boron nitride nanosheets improved dispersion while contributing additional neutron moderation capability. All fillers were processed in-house with controlled nanoscale dimensions and incorporated into High-Density Polyethylene via melt processing to fabricate a functionally graded multilayer architecture.

Radiation evaluation confirmed improved performance. At 1.0 cm thickness, gamma transmission was reduced by 27% and thermal neutron transmission by 63%. Although metallic shields offer stronger attenuation, the multilayer composite provides superior efficiency per unit mass and greater flexibility, making it promising for advanced reactors, spacecraft protection and wearable medical shielding.

Keywords: polymer nanocomposites, radiation shielding, nanoparticles

Zinc Single-Atom Nanozyme as Carbonic Anhydrase Mimic for CO_2 Capture and Conversion

Eslam M. Hamed[1], Fun Man Fung[2], Sam F. Y. Li[1*]
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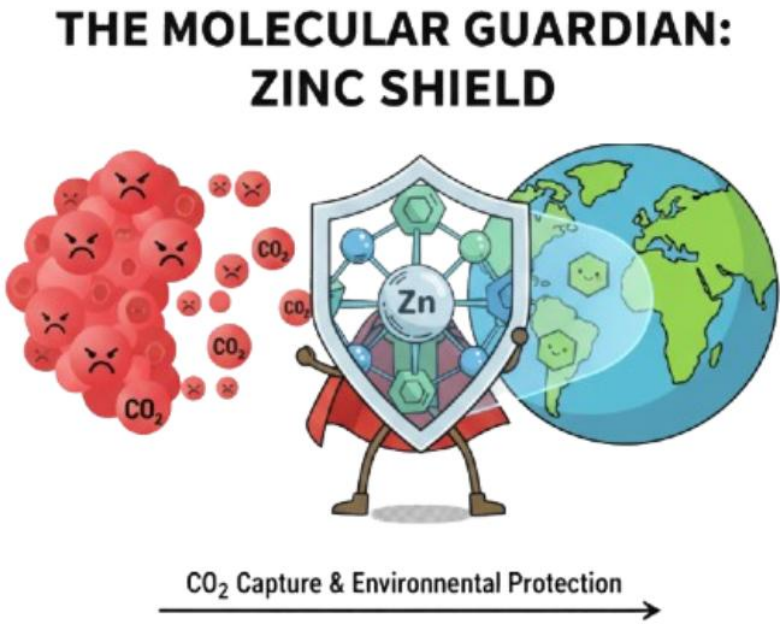
Single-atom nanozymes (SANs), with atomically dispersed metal centers, have emerged as robust, cost-effective mimics of metalloenzymes, overcoming limitations of natural enzymes such as fragility and expense. Carbonic anhydrase (CA), a zinc-based enzyme catalyzing CO_2 hydration, is highly efficient but impractical for widespread use due to its instability and high cost. Biomimetic catalysts like SANs could replicate CA's activity with improved durability and scalability.

The study aims to design a Zn-N-C SAN that emulates the active site geometry of CA to achieve efficient CO_2 capture and in-situ conversion to bicarbonate. The goals were to synthesize a high-metal-loading SAN with Zn active sites and to evaluate its CO_2 uptake and conversion efficiency.

Zn-SAN featured a distorted trigonal Zn-N_3 coordination, high thermal, pH (2-12), and solvent stability, and >18 wt % Zn loading. It achieved a CO_2 uptake of 2.3 mmol g^{-1} and converted over 91 % of adsorbed CO_2 into bicarbonate, yielding $CaCO_3$ sequestration capacity of 42 mg per mg of Zn-SAN outperforming controls. The SAN maintained high catalytic activity across cycles. Moreover, amino acids (His, Cys, Glu, Asp) inhibited catalysis by binding Zn, enabling their detection at µM-nM levels.

Keywords: Single-Atom Nanozymes; Carbonic Anhydrase; CO_2 Capture; Amino Acids



Precisely Manipulating Polymer-Chain-Interactions for Multifunctional Hydrogel

Shuai Guo [1], Swee Ching Tan[1*]
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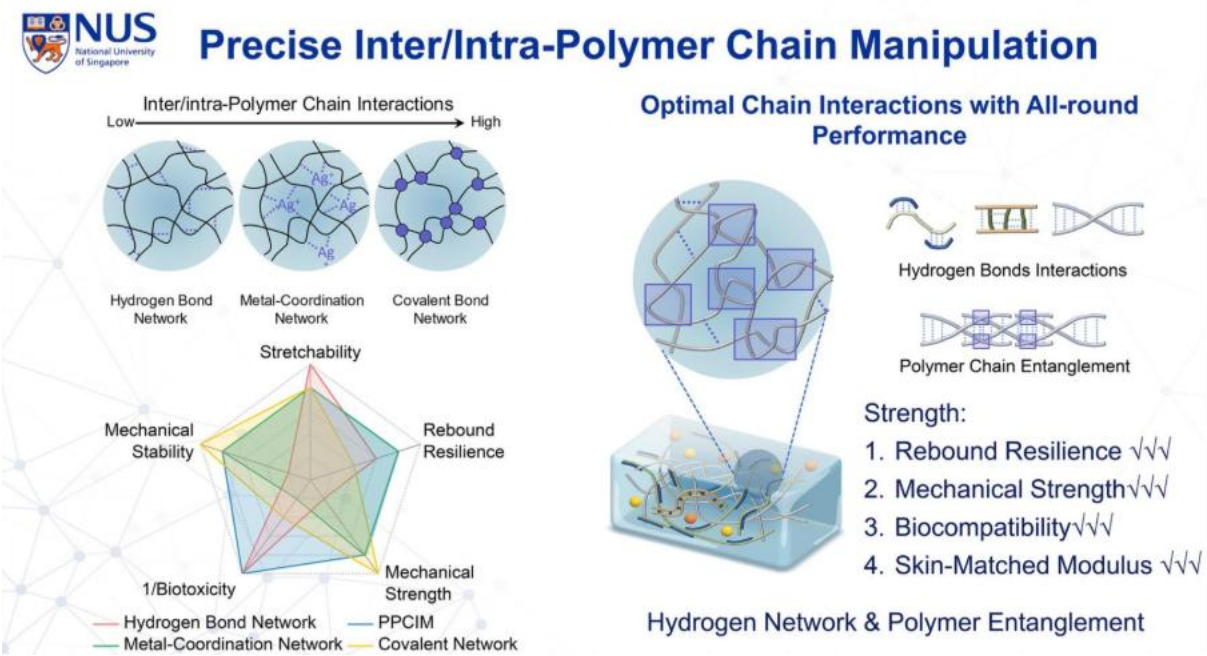
Stretchable and conductive hydrogels are essential in wearable electronics but often suffer from poor mechanical strength, large strain hysteresis, or deteriorated stability due to suboptimal polymer chain interactions. In this talk, we will deliver a precise inter/intra-polymer-chain-interaction manipulation approach that endows hydrogels with excellent performance and multifunctionality. Our hydrogels exhibit high softness (~200 kPa modulus), stretchability, conductivity, and excellent rebound resilience (energy loss coefficient <0.15). Besides, they also demonstrate excellent water retention, high conductivity, and stability at room temperature. As a self-powered tactile sensor, these hydrogels can detect large strains at high frequencies (up to 50 Hz) and tiny stimuli (~0.2% strain or 5 Pa pressure) with a fast response time (42 ms). Different from previous approaches that rely on merely one type of polymer chain interactions, the key success of our method lies in unique hydrogen bond networks and polymer chain entanglements achieved through plasticizer softening, freezing-thawing, and salt-soaking processes. We believe our approach provides a fundamental solution and valuable insights for preparing intrinsically stretchable and conductive hydrogels for versatile applications.

Keywords: wearable electronics, conductive hydrogels, interchain interactions manipulations, human-machine interactions



Benchmarking foundation potentials against quantum chemistry methods for predicting molecular redox potentials

Yicheng Chen[1], Lixue Cheng[2], Yan Jing[1], Peichen Zhong[1*]
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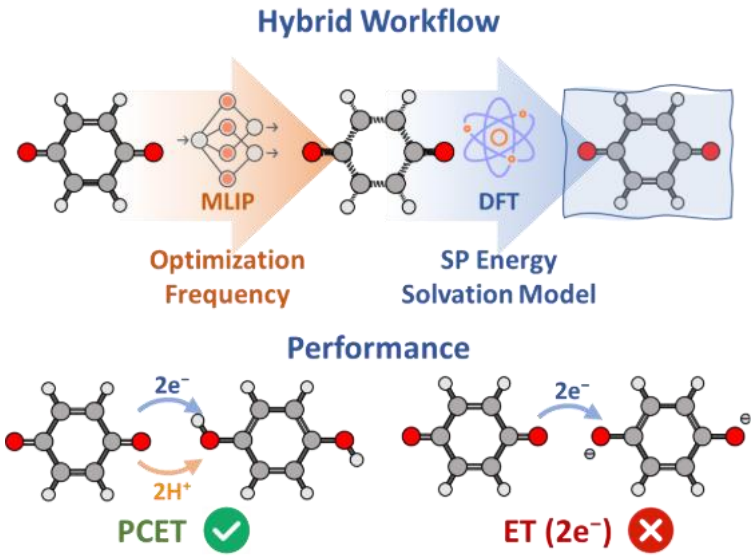
Computational high-throughput virtual screening is essential for identifying redox-active molecules for sustainable applications such as electrochemical carbon capture. A primary challenge in this approach is the high computational cost associated with accurate quantum chemistry calculations. Machine learning foundation potentials (FPs) trained on extensive density functional theory (DFT) calculations offer a computationally efficient alternative. Here, we benchmark the MACE-OMol-0 and UMA FPs against a hierarchy of DFT functionals for predicting experimental molecular redox potentials for both electron transfer (ET) and proton-coupled electron transfer (PCET) reactions. We find that these FPs achieve exceptional accuracy for PCET processes, rivaling their target DFT method. However, the performance is diminished for ET reactions, particularly for multi-electron transfers involving reactive ions that are underrepresented in the OMol25 training data, revealing a key out-of-distribution limitation. To overcome this, we propose an optimal hybrid workflow that uses the FPs for efficient geometry optimization and thermochemical analysis, followed by a crucial single-point DFT energy refinement and an implicit solvation correction. This pragmatic approach provides a robust and scalable strategy for accelerating high-throughput virtual screening in sustainable chemistry.

Keywords: Density functional theory; foundation potential; redox potential



Formulation of water-based barrier coatings for sustainable packaging

Guan Ji, Lim[1], Aqil Raziq Bin Abdul Razak[2], Teng Yih, Lee[3], Kheng Wee, Lim[4], Kay Yang, Foo[5*]
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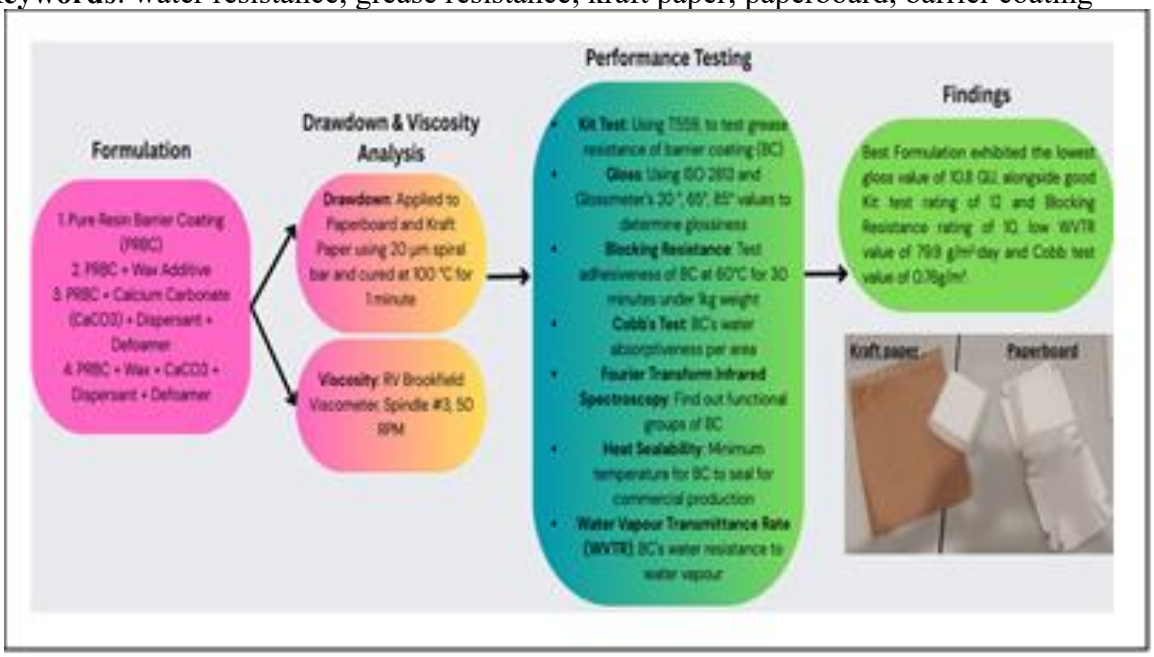
Laminated metals and plastics are widely used in food packaging but pose significant challenges in recycling due to difficulties in separating aluminum layers and segregating different plastic types. This project aims to develop water-based barrier coatings as a sustainable alternative for food packaging applications, with good barrier properties while achieving recyclability, heat sealability and surface finish compatible with customer preference. Various resin formulations were developed using different additives and barrier modifiers. The coatings were applied onto Kraft paper and paperboards, followed by performance tests including gloss measurement, grease and water resistance, and heat sealability measurements. Results show that optimal formulations with added additives (wax, dispersant and defoamer) and barrier modifier (calcium carbonate), improved water and grease resistance, produced a desirable surface finish for consumer packaging with good heat-sealing properties. This study demonstrates that water-based coatings offer a viable, environmental alternative to conventional plastic or wax-based barriers while meeting industry standards. The developed formulations also displayed water vapour barrier and grease repellency properties that outperform some commercially available high barrier paper packaging products.

Keywords: water resistance; grease resistance; kraft paper; paperboard; barrier coating



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Stimuli-activated soft actuator via ionic assembly of shear-aligned chitosan

Yuki Sum Yong Lee[1,2], Sirawit Pruksawan[1] and FuKe Wang[1,*]
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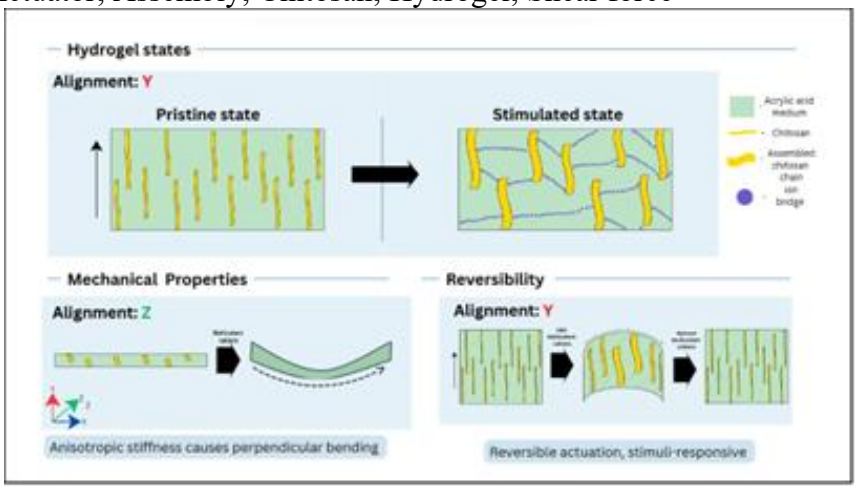
MENTOR AFFILIATIONS: AGENCY FOR SCIENCE, TECHNOLOGY AND RESEARCH (A*STAR) INSTITUTE OF MATERIALS RESEARCH AND ENGINEERING (IMRE)

A stimuli-responsive hydrogel actuator was produced by shear aligning chitosan in a poly(acrylic acid) matrix. It exhibits reversible anisotropic mechanics and perpendicular shape morphing. In the pristine state, the hydrogel demonstrates isotropic properties and a low mechanical stiffness, rendering it unsuitable for load-bearing applications. However, upon treatment with multivalent cations (eg. Ca^{2+}), the pre-aligned chitosan chains were assembled into multilevelly aligned domains triggered by reversible ionic bridging. This reinforces the hydrogel and activates its anisotropic mechanical behaviour, bringing about an increase of as much as 60 times in tensile strength and distinct anisotropic stiffness, exhibiting greater strength perpendicular to the alignment axis than along it, thereby restricting deformation along the aligned direction and driving controlled bending and morphing perpendicular to the alignment. Morphological analyses revealed alignment-preserved densification and anisotropic shrinkage upon activation, validating the mechanically driven actuation mechanism. This hydrogel system separates alignment from permanent structure, enabling reversible, stimulus-controlled mechanical anisotropy and customisable actuation without permanent fillers or multilayer systems. This hydrogel offers a scalable platform for emerging biomimetic actuators, with potential applications in soft robotics and artificial muscles.

Keywords: Actuator; Assembly; Chitosan; Hydrogel; Shear force



Enhancement of Ultraviolet Resistance of Polyaspartics Using Metal Oxide Particles

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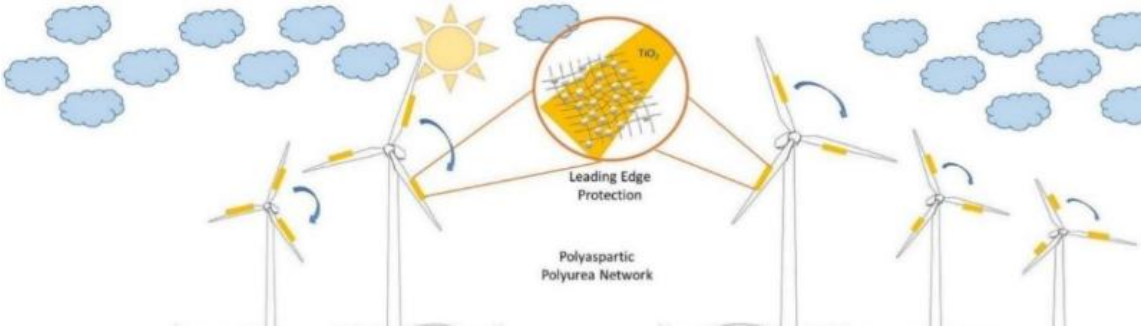
The degradation of polyaspartic ester (PAE) resins under ultraviolet (UV) radiation limits their long-term use in outdoor applications [*Polym. Adv. Technol.* 2021, 32, 8, 2797-2812]. The UV performance of these resins can be improved by incorporating metal oxide particles as UV absorbers. In this study, TiO_2 and CeO_2 particles were used to enhance the UV resistance of PAE resins. The surfaces of the metal oxides were modified with a silane coupling agent, 3-methacryloxypropyltrimethoxysilane, via a grafting method to improve their compatibility with the polymer matrix. After incorporation into the PAE resin, the UV performance of the systems was evaluated. UV-Vis spectroscopy showed that the absorbance of neat PAE resin (0.25 at 335 nm) increased to 0.47 and 0.61 with the addition of TiO_2 and CeO_2, respectively. Polyaspartic ester polyurea (PAEPU) films prepared from PAE containing 0.5, 1, and 2 wt.% metal oxides were subjected to accelerated UV weathering for 360 h. Compared to pure PAEPU ($\Delta E = 2.19$), the film containing 0.5 wt.% CeO_2 exhibited the lowest color change ($\Delta E = 0.78$). These results indicate that low TiO_2 and CeO_2 loadings in the PAE matrix enable UV-stabilized PAEPU coatings for wind turbine blade leading-edge protection.

Keywords: absorption; weathering test; scattering; UV protection; polyurea



Optimization of hydrogel sunscreen systems containing Phenylbenzimidazole Sulfonic Acid, Terephthalylidene Dicamphor Sulfonic Acid, and Disodium Phenyl Dibenzimidazole Tetrasulfonate for transparency, stability, and sensory performance

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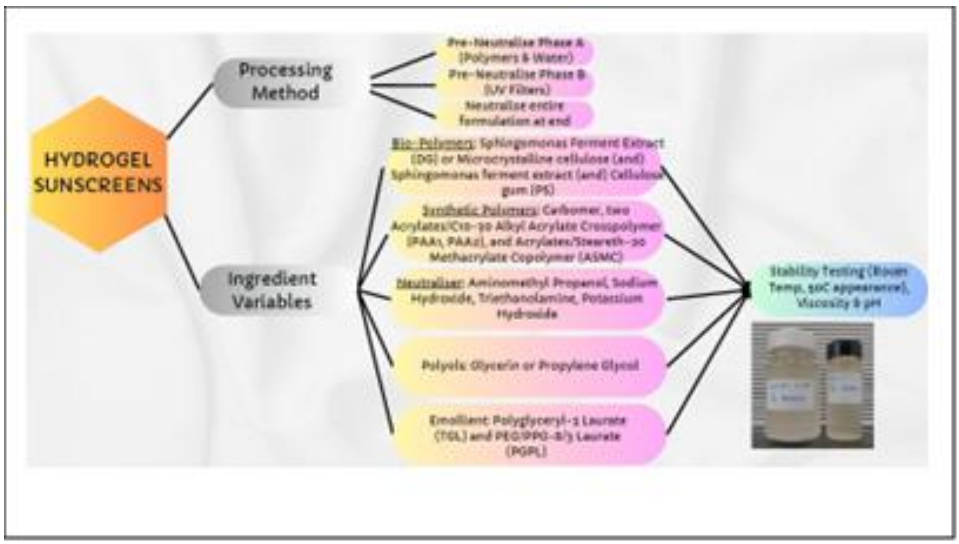
Oil-based or emulsion-based sunscreens often leave a greasy residue and/or white cast, reducing user appeal. Using hydrogel sunscreens with water soluble UV filters such as Phenylbenzimidazole Sulfonic Acid, Terephthalylidene Dicamphor Sulfonic Acid and Disodium Phenyl Dibenzimidazole Tetrasulfonate can offer a non-greasy, lightweight, and more pleasant sensory experience, while also hydrating the skin. This project explores both processing (neutralisation) and ingredient variables (i.e. stabilisers and neutralisers). It also dives into the detailed study of biopolymers, Sphingomonas Ferment Extract (DG) and Microcrystalline cellulose (and) Sphingomonas ferment extract (and) Cellulose gum; synthetic polymers of Carbomer, two Acrylates/C10-30 Alkyl Acrylate Crosspolymer (PAA1, PAA2) and Acrylates/Steareth-20 Methacrylate Copolymer; neutralisers (Aminomethyl Propanol, Sodium Hydroxide, Triethanolamine, Potassium Hydroxide); polyols (Glycerin and Propylene Glycol); and emollients Polyglyceryl-3 Laurate and PEG/PPG-8/3 Laurate, on the appearance, stability and viscosity of the hydrogel sunscreen. The objective is to optimise the formulation components and process for a transparent and gel-like sunscreen. Each formulation was subjected to stability tests, including 1 month at room and elevated temperature. Results show that the DG/PAA1 as the stabiliser system, Aminomethyl Propanol as neutraliser, Glycerin and PGPL as the humectant/emollient package, produced a transparent hydrogel with viscosity of 4000 mPa·s. and good stability under both conditions.

Keywords: sunscreen; UV filters; polymer; hydrogel; transparent



Reversible anti-fouling coating for sustainable and reusable reverse osmosis membranes

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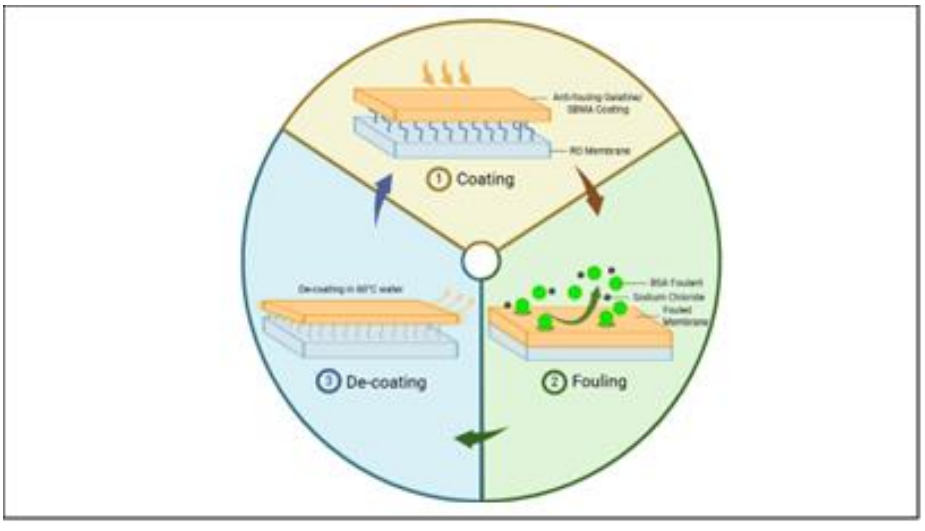
Reverse osmosis (RO) membranes are widely employed for desalination and wastewater treatment due to their high rejection of dissolved salts and contaminants. However, their operational lifetime is limited by membrane fouling, deterioration, and mechanical aging. Surface modification offers an effective strategy to enhance fouling resistance, yet most methods are permanent and difficult to regenerate once contaminated. Herein, we report a removable and re-assemblable antifouling coating for commercial RO membranes using gelatine and zwitterionic polymer sulfobetaine methacrylate (SBMA). The coating was deposited using a simple, rapid, water-based process at varying concentrations to improve membrane sustainability and reusability. The coated membranes were characterized by scanning electron microscopy (SEM), Fourier transform infrared (FTIR) spectroscopy, and water contact angle (WCA). An optimal formulation of 5 wt% gelatine and 5 wt% SBMA achieved a pure water permeance of 2.30 $L \cdot m^{-2} \cdot h^{-1} \cdot bar^{-1}$ and sodium chloride rejection of 96.4%. Importantly, the gelatine/SBMA coating was completely removed by water treatment at 60°C, recovering the original membrane surface without structural damage. The membrane was subsequently re-coated and reused, demonstrating separation performance restoration. This reversible strategy offers a sustainable approach for extending RO membrane lifespan by periodic removal and reassembly of the antifouling layer, reducing membrane replacement and waste generation.

Keywords: RO Membrane; Anti-fouling; Sustainability; Gelatine; SBMA



Uncertainty-Aware Machine-Learning Active Learning for Screening Lead-Free Halide Perovskites

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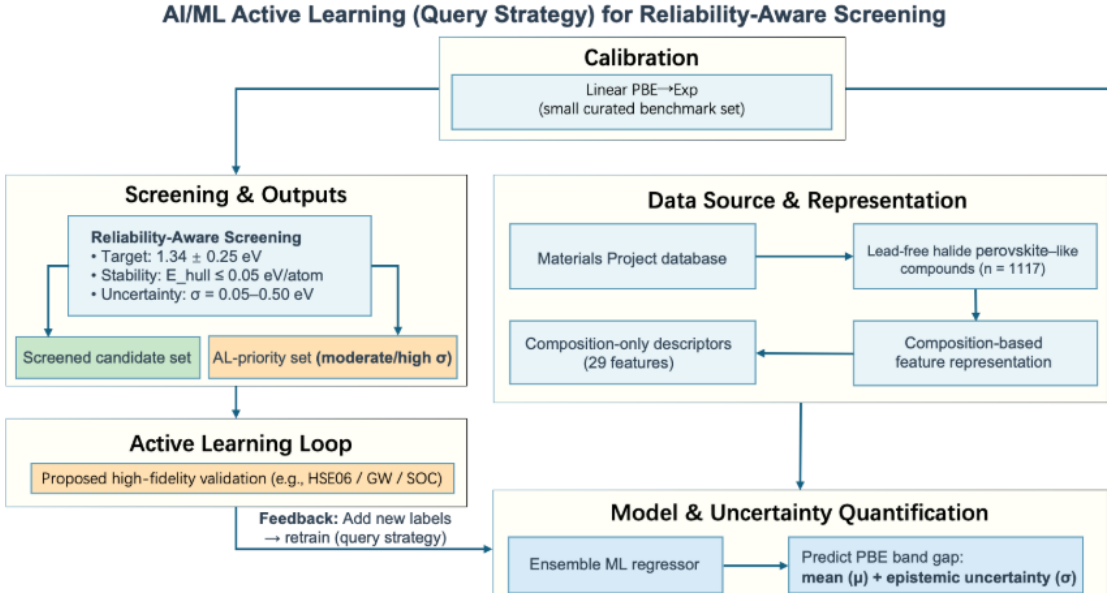
The rapid growth of machine learning–assisted materials screening has enabled the exploration of vast chemical spaces with unprecedented efficiency. However, conventional workflows often treat all model predictions as equally reliable, leading to "blind confidence" when extrapolating to novel materials. In this work, we develop an uncertainty-aware active learning framework for screening lead-free halide perovskites for photovoltaic applications, explicitly distinguishing reliable predictions from regions of limited model knowledge. Instead of restricting the search to ideal cubic perovskites, we include distorted, vacancy-ordered, and mixed-anion structures to reflect the structural diversity of lead-free systems. An ensemble regression model predicts DFT band gaps while quantifying epistemic uncertainty arising from data sparsity and model disagreement.

To address systematic band gap underestimation by semi-local functionals like PBE, we apply a statistically validated, stratified calibration scheme using experimentally characterized benchmarks. This aligns predicted trends with observations without artificially inflating accuracy. Screening reveals recurring chemical motifs, including heavy d-electron halides, identified as potential false positives from known functional limitations and composition-based feature abstractions. Rather than claiming definitive discoveries, this study shows how uncertainty quantification and active learning expose blind spots in conventional screening pipelines and guide prioritization of 121 high-uncertainty, physically promising candidates for higher-fidelity calculations.

Keywords: perovskite materials; active learning; machine learning; bandgap prediction; uncertainty quantification



ACS Chapter Singapore

A Hybrid Physics-Driven Neural Network Force Field for Liquid Electrolytes

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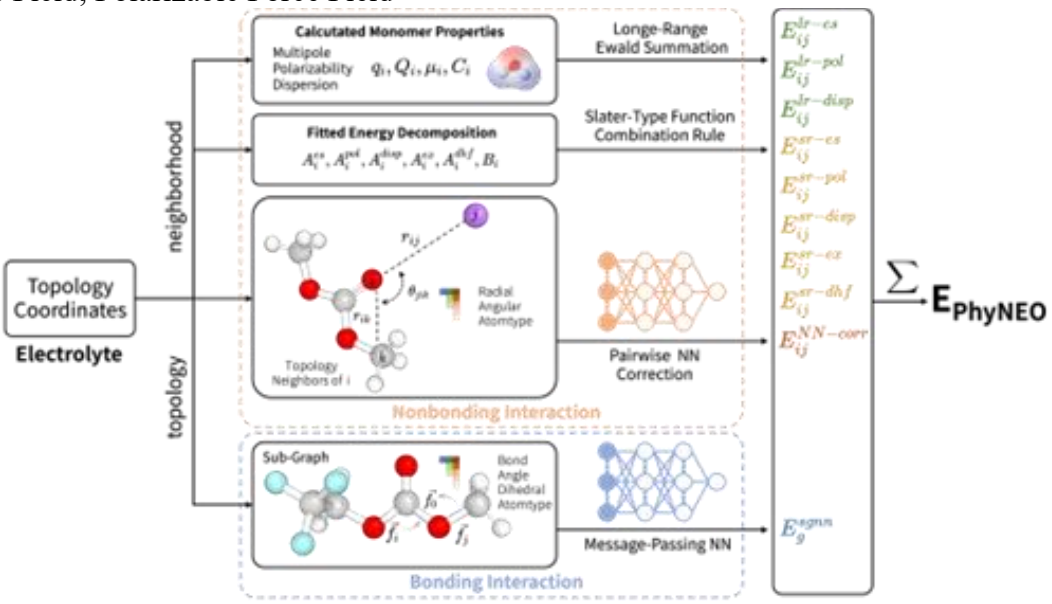
Machine-learning force fields (MLFFs) are rapidly transforming molecular dynamics (MD) simulations. However, MLFFs still face challenges, particularly in accurately describing long-range interactions and maintaining computational efficiency, which significantly limits their application to non-periodic systems like electrolytes and polymers. In this work, we introduce PhyNEO-Electrolyte (Physics-Driven and Neural Network Enhanced Organic Force Field for Electrolytes), a fully ab initio, differentiable force field designed for practical lithium and potential sodium battery electrolytes. By employing a range-separation scheme, we effectively capture long-range electrostatics, dispersion, and polarization interactions, while significantly improving short-range fitting through a natural pairwise machine-learning framework. Additionally, bonding interactions are modeled using a topologically localized sub-graph neural network. This approach enables the construction of an efficient and scalable electrolyte force field that spans a broad chemical space, from small monomers and dimers to larger systems, providing high accuracy in both microscopic and macroscopic properties of interest to experimental scientists. We hope our force field will inspire further efforts toward developing a general molecular force field.

Keywords: Machine Learning Force Field; Electrolyte; Molecular Dynamics Simulation; Force Field; Polarizable Force Field



Selective electrochemical oxidation of primary alcohols to aldehydes in organic electrolytes

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Conventional oxidation of primary alcohols to aldehydes typically relies on toxic oxidants, while greener alternatives such as electrochemical oxidation often suffer from over-oxidation to carboxylic acids. Here, we report a simple electrochemical method for the selective oxidation of primary alcohols to aldehydes. Using commercially available electrodes under potentiostatic control in organic electrolytes, we systematically investigate the oxidation behaviour of a range of primary alcohols. The method achieves high aldehyde selectivity with faradaic efficiency exceeding 90% and no detectable carboxylic acid by-products as confirmed by HPLC-UV analysis. Operating at ambient temperature and without stoichiometric chemical oxidants, this approach offers an environmentally benign route to aldehyde synthesis in line with the principles of green chemistry.

Keywords: Electrochemical oxidation; primary alcohols; aldehydes; green chemistry

Edge Functionalisation of Curved Nanographenes

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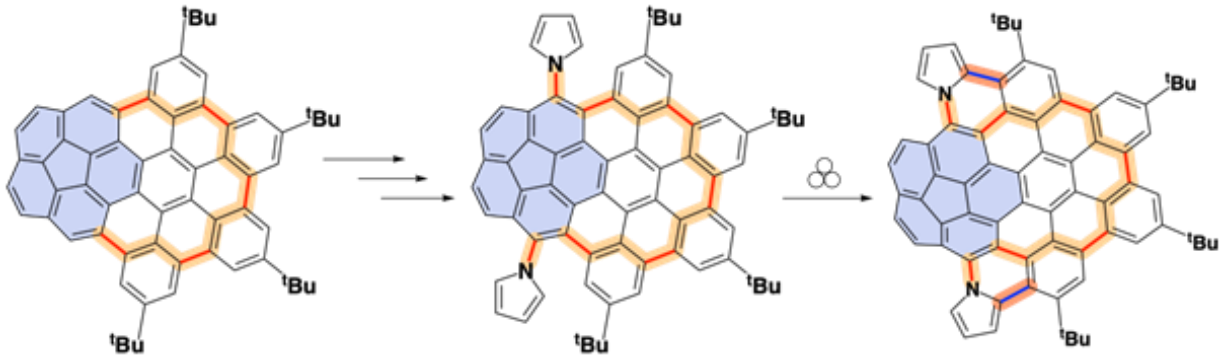
In this work, the extension of curved aromatic systems based on a corannulene–coronene hybrid is explored through direct edge functionalization strategies. This hybrid nanographene, constructed via a bottom-up synthetic approach, provides a unique platform in which molecular curvature and extended π-conjugation coexist within a single framework. Regioselective aromatic substitution reactions will be employed to functionalize the peripheral edge sites of the curved nanographene, enabling controlled modification of its electronic and structural features.

The introduced functionalities are expected to influence local aromaticity and reactivity while serving as precursors for subsequent intramolecular fusion reactions. These fusion processes will further extend the π-conjugated network, enhancing aromatization and promoting partial graphitization of the molecular framework. The resulting enlarged curved π-systems are anticipated to exhibit modified electronic structures and optical responses.

By systematically extending conjugation and curvature, this study aims to establish structure–property relationships in curved nanographenes, with particular emphasis on the evolution of optical absorption and emission characteristics.

Keywords: Curved Nanographenes; corannulene; aromatization; nucleophilic substitution



Forced degradation of a block copolymer to guide stability considerations in polymeric nanoparticle formulation development

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ACM Biolabs utilizes an amphiphilic block copolymer (ABC) in its research and development of block copolymer nanoparticle (BNP) formulations for drug delivery applications. The stability of polymeric excipients is critical for the development of robust BNP formulations. In this study, ABC was subjected to controlled stress conditions, as recommended by International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH) Q1A (R2) and Q1B guidelines, to evaluate its susceptibility to degradation. The extent of degradation was quantified using gel permeation chromatography (GPC), while the structures of the resulting degradation products were characterized by proton nuclear magnetic resonance spectroscopy. Stress studies indicate that the ABC is susceptible to thermal, oxidative, and photolytic exposure, and its degradation proceeds in a kinetically controlled manner. GPC chromatogram showed a front-shoulder peak under these conditions, indicating the formation of higher-molecular-weight species. This was attributed to radical generation, where radicals either react with oxygen to form peroxides and epoxide groups or recombine with radicals on neighboring chains, leading to crosslinking. To minimize the formation of oxidative and photolytic impurities, the ABC is stored at sub-ambient temperature, under an inert atmosphere, and protected from light, translating to the storage conditions for polymeric nanoparticle formulations.

Keywords: Stress degradation; stability; block copolymer nanoparticles; drug excipient

Motif-driven scalable design of rutile high-entropy oxide catalysts for oxygen evolution reaction

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The discovery of efficient rutile high-entropy oxide (HEO) catalysts for oxygen evolution reaction (OER) is limited by the combinatorial expansion of compositional diversity, surface heterogeneity, and site-dependent OER pathways, which make brute-force density functional theory (DFT) enumeration impractical. Here, we develop a motif-based analytical framework that enables scalable prediction of adsorption energetics on rutile-type HEO surfaces. Using a systematic DFT dataset, we show that conventional scaling relations break down intrinsically as adsorption energies remain widely dispersed even when the active-center element is fixed. We then apply physically constrained multitask symbolic regression to derive a unified analytical expression that predicts the adsorption energies of *O, *OH, and *OOH intermediates from elemental physicochemical properties and local coordination motifs. This analytical model enables zero-DFT-cost prediction of overpotential and pathway preference across vast compositional spaces. Cost-performance Pareto screening identifies rutile low-Ru oxides with enhanced predicted activity, and experiments on representative compositions validate these trends. Together, this work establishes an interpretable and transferable strategy for scalable oxide-catalyst design beyond brute-force DFT calculations.

Keywords: scalable design; high entropy oxide; oxygen evolution reaction

Investigating the use of a hybrid Fmoc-D-Phe-alginate hydrogel as a drug delivery medium for wound-related pain treatment

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The feasibility of a new hydrogel synthesised from Fmoc-D-Phe amino acid and alginate polymers is investigated as a low-cost and low-complexity drug delivery medium for wound-related pain treatment. The use of hydrogels as drug-delivery mediums is effective due to their ability to provide localised drug entrapment and controlled release behaviour. By cross-linking the self-assembling Fmoc-D-Phe with sodium alginate and $CaCl_2$ solution, a stable hybrid hydrogel with improved drug delivery kinetics and water retention is formed. The single amino acid structure of Fmoc-D-Phe provides a porous structural network due to its absence of compact β-sheet formation, facilitating more rapid diffusion of the encapsulated analgesic. The incorporation of alginate increases the mechanical strength of the structure, while its hydrated domains further improve drug delivery kinetics by lowering diffusion tortuosity. These results demonstrate that this hybrid system is suitable as a material platform for wound-related pain treatment due to controlled burst release of the drug and its initial buffering phase. Furthermore, these properties also enable rapid release profiles associated with fast onset analgesic delivery for patients while mitigating the likelihood of localized irritation that can arise from abrupt elevations in drug concentration.

Keywords: self-assembling peptide hydrogel, Fmoc-amino acid, alginate cross-linking, hybrid hydrogel network, burst release profile

ACS Chapter Singapore

Shear-aligned bioprinting of chitosan hydrogels for programmable, multidirectional actuation

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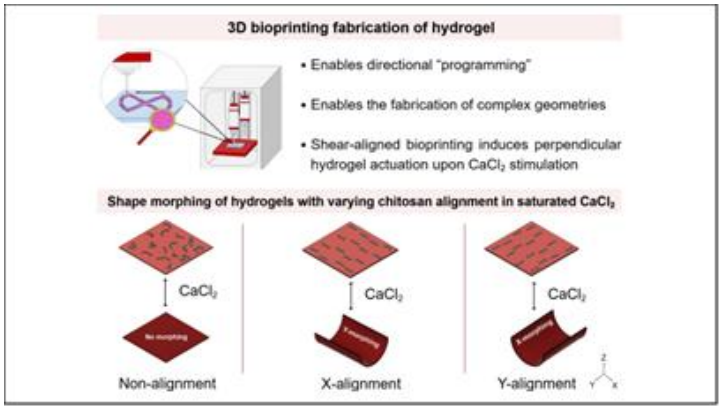
Hydrogel-based soft actuators commonly rely on anisotropic structures or indirect swelling to induce motion, limiting reversibility and design flexibility. Extrusion-based 3D printing enables the fabrication of complex geometries, yet achieving predictable, reversible anisotropic actuation without permanent fillers remains challenging. Here, a shear-aligned chitosan (CS) hydrogel actuator in which anisotropic shape morphing is done directly through extrusion-based bioprinting. As the hydrogel precursor is extruded through the nozzle, shear flow aligns CS chains along the printing direction, and subsequent saturated $CaCl_2$ immersion induces actuation. Directional stiffening restricts deformation along the printing direction, causing bending perpendicular to alignment. Complex geometries – crosses, four-leaf clovers – exhibit morphing that initiates with perpendicular bending and evolves into curling or twisting depending on geometry. By varying printing orientations within a structure, distinct and localised actuation are achieved, demonstrated by a flower-like geometry with petals curling in opposite directions. Finite element analysis accurately predicts these behaviours. Notably, the hydrogels function as stiffness-adaptive graspers, simultaneously morphing and increasing toughness by up to ~350-fold to securely grip objects, before reversibly softening upon stimulus removal. With this, it enables programmable, multidirectional hydrogel actuation for advanced soft robotics and biomedical applications.

Keywords: 3D bioprinting; Hydrogel; Multidirectional morphing; Shear align; Chitosan



Controlling evaporation driven growth of single crystals as a model for chiral materials

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In this study, we present a multistage, evaporation-based protocol for growing fully transparent 1x1 cm sodium chloride (NaCl) single crystals. In Stage 1, we form 3x3 mm cubic seeds under controlled supersaturation; in Stage 2, these seeds are scaled to centimetre dimensions while minimising secondary nucleation and defect formation. Two recurring challenges are (i) obtaining uniformly cubic seeds and (ii) preserving optical transparency during crystal growth. Our observations implicate excessively rapid evaporation, airborne particulate contamination, and uncontrolled airflow as primary sources of morphological irregularities and light-scattering inclusions.
To address these challenges, we compare (a) solution ageing to equilibrate supersaturation and reduce spontaneous nucleation, (b) fine filtration and clean handling to remove dust and heterogeneous nuclei, and (c) humidity buffered, airtight enclosures to stabilise local vapour pressure and suppress convective gradients. Preliminary trials using a 3L beaker on perforated staging indicate that airflow and tissue substrates introduce heterogeneous nucleation sites; transitioning to sealed chambers, inert substrates, and gentle vapour phase control is expected to reduce defect density and improve clarity. Results suggest that this protocol for growing large, transparent NaCl crystals suitable for optics demonstrations is appropriate and could potentially be used as a methodology to grow chiral compounds with tunable optoelectronic properties.

Keywords: sodium chloride; seed growth; controlled evaporation; transparency; nucleation control.

Chitosan-Induced Rapid and Controllable Hydrogel Degradation for Biomedical Uses

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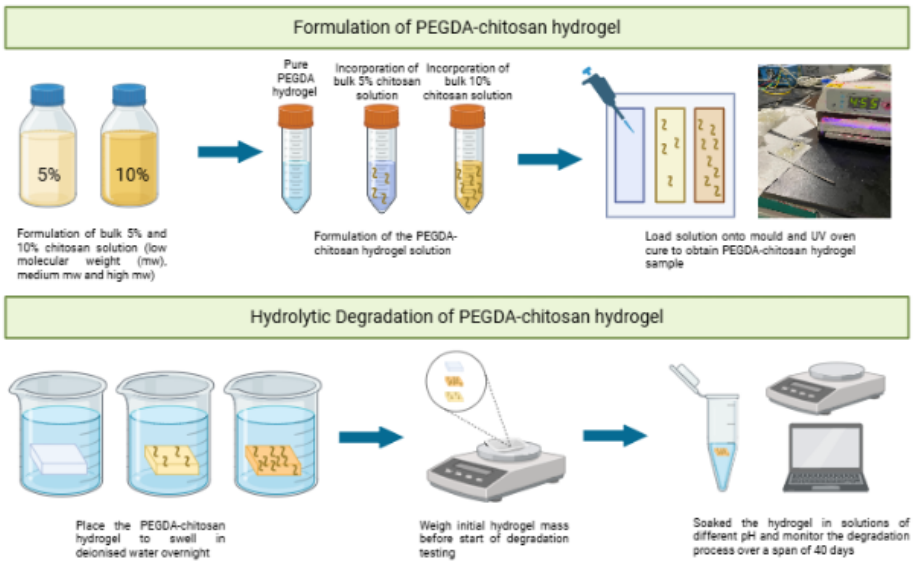
Hydrogels are widely employed in biomedical and engineering applications due to their tunable chemical, mechanical, and biological properties. However, many hydrogel systems exhibit relatively slow degradation, limiting their effectiveness in applications that rely on timely degradation, such as regenerative medicine, drug delivery, and tissue engineering. Therefore, proposing strategies that enable accelerated and controllable hydrogel degradation are desirable. In this study, a poly(ethylene glycol) diacrylate (PEGDA)-based hydrogel system was used as the matrix, with chitosan incorporated as a degradation accelerator and regulator, to investigate the effects of hydrogel composition and environmental pH on hydrolytic degradation behavior. PEGDA-chitosan hydrogels were synthesized and systematically evaluated to evaluate the effects of solution pH and chitosan molecular weight on biodegradation behavior. The results showed that incorporating chitosan significantly accelerated PEGDA hydrogel degradation compared to pure PEGDA hydrogel across all pH conditions, with the highest degradation observed at lower pH values, and higher molecular weight chitosan producing a greater extent of degradation.

Keywords: Degradation; Chitosan; Hydrogel; pH



Aldehyde quantification using novel fluorometric assay of Galactose Oxidase activity

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Biocatalysis employs enzymes to enable highly selective chemical transformations under mild conditions, reducing energy needs, waste, and use of hazardous reagents in chemical manufacturing. Our lab developed mutants of galactose oxidase, an enzyme that oxidises alcohols, with the goal to develop a mutant that would selectively oxidise primary alcohols in diol substrates. However, current analytical assays for alcohol oxidation largely quantify total oxidation, providing limited ability to selectively assess primary alcohol oxidation. Here, we develop a fluorometric Hantzsch-based assay enabling selective quantification of aldehydes, to allow us to assess the extent of primary alcohol oxidation. It has a limit of detection of 0.01 mM and a limit of quantification of 0.04 mM. The assay's fluorometric response is linear, with a R^2 value of 0.9996. This assay is fast, taking 30 minutes of incubation time and is user-friendly, enabling scalable high-throughput screening of enzyme variants toward precision oxidation. We envision that our assay can be employed to develop more efficient, cost-effective, and sustainable synthetic routes through biocatalytic reactions, reducing undesirable byproducts. These routes could be for high-value specialty chemicals containing aldehydes such as those from the pharmaceutical or flavour industries.

Keywords: assay; fluorometry; Hantzch reaction; aldehyde; galactose oxidase

Synthesis of Extended Nanographenes

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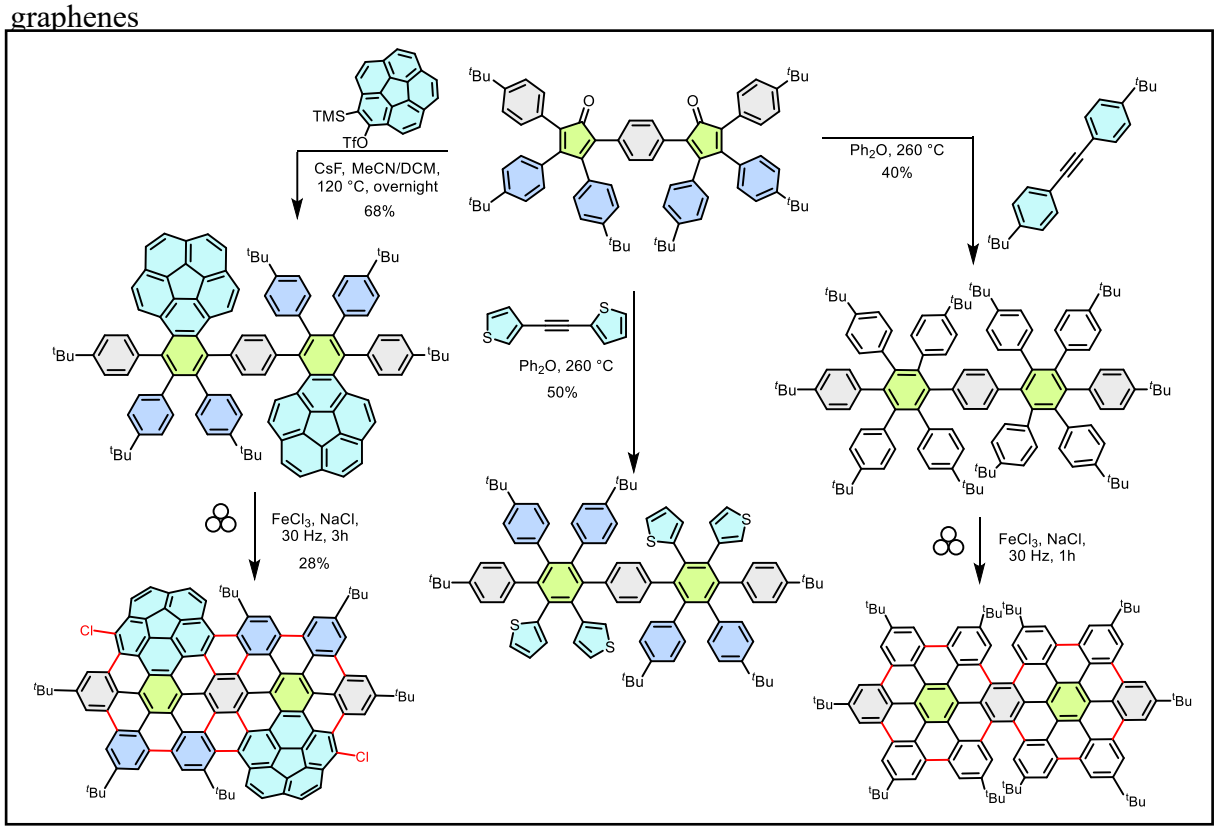
Nanographenes have attracted considerable interest as functional molecular materials due to their potential applications in organic photovoltaics, light-emitting devices, organic field-effect transistors, host–guest systems, polymeric materials, and chemical sensing. Their structural diversity and tunable electronic properties make them an important class of π-conjugated systems in contemporary materials chemistry.
In this study, curved and π-extended nanographene frameworks were constructed through a sequence of cycloaddition and oxidative cyclization reactions. Diels–Alder reactions involving cyclopentadienone-based building blocks were employed as a key strategy for assembling larger nonplanar architectures, with bis-cyclopentadienone intermediate enabling framework growth. To further increase structural complexity, a tris-cyclopentadienone precursor was synthesized for higher-order nanographene formation. Subsequent Scholl reactions led to the formation of a corannulene–coronene dimer, in which the anti-diastereomer was obtained preferentially—an interesting stereochemical outcome that should be further investigated.

Keywords: nanographenes; corannulene; mechanochemical synthesis; curved molecular graphenes



Controls on trace metal accumulation in mangrove sediments of Singapore: Implications for coastal ecosystem management

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Mangroves are vital coastal buffers and biodiversity hotspots; however, they are vulnerable to trace-metal contamination that alter sediment geochemistry and metal bioavailability, affecting ecosystem function. This study investigates trace-metal distributions and sediment characteristics in the mangroves of Pulau Ubin, an area subject to low-to-moderate anthropogenic influence associated with coastal activities and historical land use. Surface sediments and sediment cores were collected across Ubin to examine both spatial variability and downcore changes in sediment composition. Particle-size analysis was conducted to characterise properties that influence metal binding and bioavailability. Trace-metal concentrations were quantified using Inductively Coupled Plasma–Mass Spectrometry (ICP-MS) following acid digestion, while total organic carbon and nitrogen were measured to explore links between organic matter, grain size, and metal retention. Stable isotope analysis ($\delta^{13}C$ and $\delta^{15}N$) will used to support interpretation of organic-matter sources and shifts in trophic dynamics. This study aims to distinguish natural background signatures from anthropogenic inputs and to assess how sediment properties regulate contaminant behaviour. The results will provide a contemporary geochemical baseline for Pulau Ubin mangroves, enabling comparison between northern and southern sites as well as across depths. Ultimately, these findings will contribute to ecological risk assessment and inform management of mangrove habitats in Singapore.

Keywords: Mangrove sediments; Trace metals; Anthropogenic influence; Singapore

Bio-based microgels as a sustainable delivery system for phosphate fertilizers

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Current phosphate fertilizers found in the market have high dissolution rates, resulting in low nutrient use efficiency through processes like phosphate leaching or surface runoff. Controlled-release fertilizers (CRFs) can improve nutrient use efficiency but are often made of non-biodegradable material, which can cause environmental harm. Hence, there is a required shift to more environmentally friendly materials such as bio-based microgels with the ability to facilitate the slow release of water, enabling them to be a potential candidate for trapping phosphates in the form of monoammonium phosphate (MAP). The molybdenum blue reagent , along with a UV-Vis spectrophotometer at absorbance wavelength of 880nm, was used for both qualitative and quantitative evaluation of the uptake and subsequent release of MAP in our microgels formulation, RetenSol-G. Test results showed that RetenSol-G could retain MAP equivalent to 76% of its own mass and showed potential of controlled release.

Keywords: Controlled-release fertilizers; Sustainable agriculture; Microgel

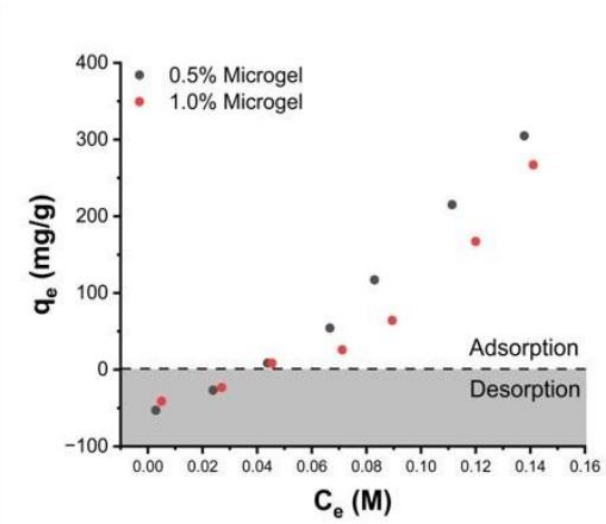

Figure 1:Successful Adsorption of MAP by microgels at varying concentrations

Profiling of nutraceuticals in stingless bee propolis extract using UV spectroscopy and GC-MS

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This study compared two stingless bee propolis samples, Propolis Sibolga Baru and Propolis Standar Baru, produced by *Geniotrigona thoracica* bees from different geographical sources, to evaluate their antioxidant potential and bioactive compounds relevant to hemorrhagic stroke management. Antioxidant capacity and chemical profiles were assessed through total phenolic content (TPC), total flavonoid content (TFC), and gas chromatography–mass spectrometry (GC–MS), providing a reliable basis for comparison between propolis sources. TPC and TFC were determined using the Folin–Ciocalteu and aluminium chloride methods, respectively, with potassium acetate (PA) included to enhance flavonoid detection, while GC–MS was used to identify volatile bioactive compounds extracted using different solvent systems. Quantitative results showed that Propolis Sibolga Baru exhibited higher TPC and TFC than Propolis Standar Baru, indicating stronger antioxidant capacity. PA increased TFC yield in Propolis Sibolga Baru but reduced yield in Propolis Standar Baru, demonstrating a source-dependent effect. GC–MS analysis identified multiple compounds associated with antioxidant and neuroprotective activity, with ethyl acetate–hexane (75:25, v/v) giving the highest extraction yield. Overall, Propolis Sibolga Baru demonstrated superior antioxidant performance, consistent with literature on the neuroprotective potential of *Geniotrigona thoracica* propolis.[1]

1. Tandean, S.; *et al.* Chemical Composition and Neuroprotective Properties of Indonesian Stingless Bee (*Geniotrigona thoracica*) Propolis Extract in an In Vivo Model of Intracerebral Hemorrhage (ICH). *Nutrients* **2024**, *16* (12), 1880. https://doi.org/10.3390/nu16121880

Keywords: Propolis; Antioxidant Properties; Total Flavonoid Content (TFC); Total Phenolic Content (TPC); Gas Chromatography-Mass Spectroscopy (GC-MS); Bioactive Compounds; Hemorrhagic Stroke

Tunable Ru PNP catalysts for the hydrogenation of carbon dioxide to methanol

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Given the potential of carbon dioxide (CO_2) hydrogenation for carbon capture and utilization [*Acc. Chem. Res.* 2019, 52 (10), 2892–2903], together with the production of platform chemicals [*ACS Catal.* 2020, 10 (19), 11318–11345], the development of homogeneous catalysts to promote the reaction under mild conditions has been flourishing in recent years [*Angew. Chem. Int. Ed.* 2022, 61 (42), e202207278]. However, the advancement of homogeneous catalysis for CO_2 hydrogenation to methanol (CO_2→MeOH) has been slower due to its complicated mechanisms, posing kinetic and compatibility challenges [*Angew. Chem. Int. Ed.* 2022, 61 (42), e202207278]. Herein, a systematic study is designed to fine-tune the electronic property of ruthenium catalysts bearing a tridentate ligand PNP (Ru PNP) to improve catalytic activity in CO_2→MeOH. Ru PNP complexes with varying phosphorus substituents were synthesized; their electronic properties were quantified by the hydride chemical shift (δ(Ru-*H*)). The trend in catalytic activity is consistent with the proposed mechanism reported in the literature [*J. Am. Chem. Soc.* 2019, 141 (7), 3160-3170]. Specifically, catalysts that are neither too electron-rich nor electron-poor performed best in CO_2→MeOH. This work has demonstrated that δ(Ru-*H*) may serve as a predictor for catalyst performance and may aid in designing more active catalysts.

Keywords: sustainability; catalysis; hydrogenation; carbon dioxide; Ru PNP

Chemical fate of carbon and nutrients during sustainable microalgal growth in palm oil mill effluent.

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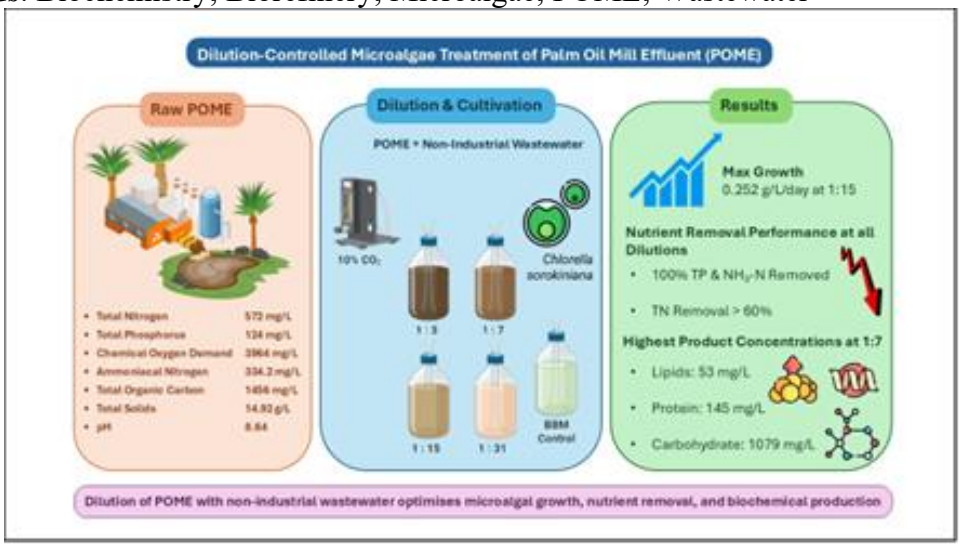
Excess carbon and nutrient loadings in palm oil mill effluent (POME) limit its use in microalgal systems, motivating the examination of carbon and nutrient fate during POME blending with non-industrial wastewater to reduce freshwater demand. Batch cultivations of *Chlorella sorokiniana* were conducted under 10% CO_2 aeration using four POME-wastewater dilution ratios and a BBM control. All wastewater samples, before and after treatment, were characterised using APHA- and USEPA-standardised analytical methods. POME contained high concentrations of TN, TP, NH_3-N, COD, and TOC, exceeding optimal limits for microalgal growth and necessitating dilution. Dilution significantly enhanced growth, with the highest growth rate observed at a 1:15 dilution (0.252 ± 0.002 g L^{-1} d^{-1}), exceeding the BBM control (0.115 ± 0.007 g L^{-1} d^{-1}). Complete removal of TP and NH_3-N was achieved in all dilutions, while TN removal exceeded 60%. Biochemical composition varied with dilution, with maximum lipid (53 ± 16 mg L^{-1}), protein (145 ± 1 mg L^{-1}), and carbohydrate (1079 ± 106 mg L^{-1}) contents at 1:7 dilution, while chlorophyll a (47.8 ± 2.4 mg L^{-1}) and b (109.3 ± 6.2 mg L^{-1}) peaked at 1:15. These results demonstrate dilution-controlled optimisation of microalgal systems for biomass growth and biorefinery applications.

Keywords: Biochemistry; Biorefinery; Microalgae; POME; Wastewater



Discovery of bioactive peptidoglycan fragments from *Lactobacillaceae* that confer intestinal protection in hosts

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Gut bacteria-derived peptidoglycan fragments (PGNs) are key signaling molecules in mammalian hosts. However, the production and functional roles of soluble PGNs secreted by individual gut bacterial species have not been systematically explored. Herein, we used a targeted LC-MS/MS approach to profile PGNs released by bacteria, identifying *Lactobacillaceae* as the predominant producers of disaccharide PGNs in culture supernatants. We then chemically synthesized such disaccharide PGNs and confirmed their activation of the mammalian sensor NOD2. Notably, priming murine macrophages with disaccharide PGNs induced tolerance to subsequent stimulation by TLR2/4 ligands, suggesting that sustained exposure to bioactive PGNs in the gut may shape host immune responses. Consistently, administration of the disaccharide PGN, GM-AQK, effectively alleviated gut inflammation in a DSS-induced colitis mouse model. Together, these findings deepen our understanding of PGN mediated gut microbiota-host crosstalk and position natural disaccharide PGNs as promising postbiotic candidates for therapeutic modulation of intestinal inflammation.

Keywords: *Lactobacilliaceae*-derived peptidoglycan fragments; LC-MS/MS; NOD2 signaling; immune tolerance; intestinal protection

Polymerizable Deep Eutectic Solvents for Simultaneous Cellulose Nanofibrillation and In-Situ Polymerization

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This study presents an environmentally conscious approach that integrates sustainability into both material selection and manufacturing processes. A ternary deep eutectic solvent (DES) system comprising choline chloride, citric acid, and acrylic acid was employed to enable simultaneous cellulose nanofibrillation and polymerization through a one-pot process, significantly reducing waste and eliminating additional processing steps typically required in conventional cellulose nanofiber isolation. The polymerizable DES system effectively facilitates biomass nanofibrillation, yielding fibrils with diameters in the range of 1–30 nm while preserving the crystalline structure of cellulose. The formation of stable biomass-containing dispersions is further supported by esterification of cellulose hydroxyl groups during treatment. Incorporation of cellulose-based biomass further demonstrate shear-thinning behavior to the composite, which is essential for direct ink writing (DIW) 3D printing of complex structures. Moreover, in situ polymerization of acrylic monomers produces soft, viscoelastic eutectogels with inherent self-adhesive, anti-freezing properties, highlighting the system's strong potential for sustainable, sensor-based applications.

Keywords: cellulose; nanofibers; eutectogels; 3D printing; anti-freezing

Fully Cyclized Corannulene-Based Curved Nanographenes: Structural Elucidation and Optimized Synthesis

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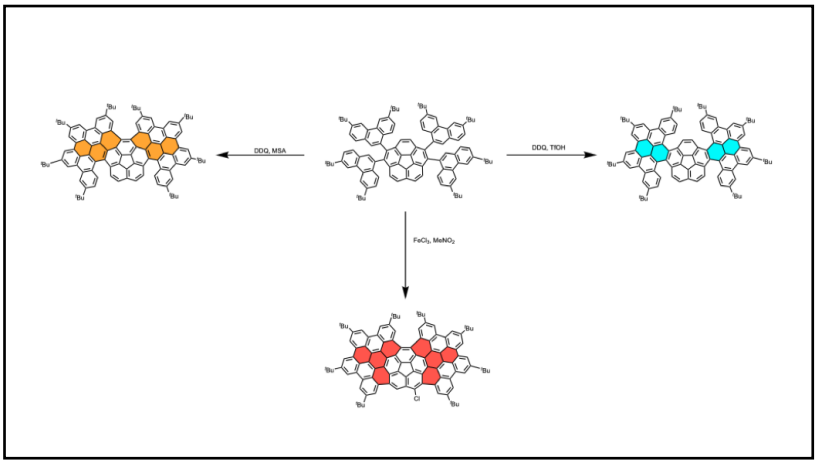
Graphene has attracted immense attention over the past decade for its exceptional electrical and mechanical properties. [*Sci*. 2008, *321*, 385-388]However, its absence of an intrinsic band gap restricts its use in semiconducting devices.[*Chem. Soc. Rev.* 2015, *44*, 6616–6643] To address this, nanographenes—finite graphene fragments with defined edges and structural defects—have been developed. [*Angew. Chem. Int. Ed.* 2018, 57, 6774-6779] Incorporating non-hexagonal rings, such as pentagons, introduces curvature and tunes electronic properties.[*Chem. Sci*. 2021, 12, 8048–8057]

Corannulene, a bowl-shaped "buckybowl" molecule, offers a promising scaffold for the bottom-up synthesis of curved nanographenes. [*Acc. Chem. Res.* 2021, 54, 2858–2870.] A key intermediate, tetrabromocorannulene, provides reactive sites for carbon–carbon coupling and Scholl reactions to extend π-conjugation. This work presents a bottom-up strategy for constructing corannulene-based curved nanographenes and investigates their electronic properties, advancing the design of functional curved π-systems for electronic and photonic applications.

Keywords: polyaromatics, corannulene, curved nanographene, nanographene synthesis, ring formation



ACS Chapter Singapore

Machine learning-based SERS chemical space for two-way prediction of structures and spectra of untrained molecules

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Identifying unknown molecules beyond existing databases remains challenging in surface-enhanced Raman scattering (SERS) spectroscopy. Conventional SERS analysis relies on matching experimental and cataloged spectra, limiting identification to known molecules. Given the vast chemical space (>10^{60} molecules), it is impractical to obtain the spectra of every molecule and rely solely on in silico techniques for spectral predictions. Here, we showcase a machine learning (ML)-based SERS chemical space that leverages spectra-structure correlations for two-way spectra-to-structure and structure-to-spectra predictions of untrained molecules [*J. Am. Chem. Soc.* 2025, 147, 8, 6654–6664]. Using a SERS chemical space comprising 38 linear molecules from four functional group classes, our experimental and in silico studies reveal key underlying spectral features that enable the prediction of untrained molecules represented by two molecular descriptors (functional group and carbon chain length). We devise a two-step "classification and regression" ML framework to sequentially predict the functional group and carbon chain length of untrained molecules with 100% accuracy and ≤1 carbon difference. Using an eXtreme Gradient Boosting regressor trained on the two descriptors, we attain inverse structure-to-spectra prediction with an average cosine similarity of 90.4% between the predicted and experimental spectra. Our ML-based SERS chemical space represents a shift for molecular identification from spectral matching to predictive modeling of spectra−structure relationships.

Keywords: surface-enhanced Raman scattering spectroscopy; chemical space; functional group; machine learning

Engineering Waste-Derived Silicate Activators for High-Performance and Scalable Geopolymer Concrete

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The dependence of geopolymer technology on conventional sodium silicate (Na_2SiO_3) activators is widely recognized as undermining its environmental and economic advantages. In this study, a chemistry-driven strategy was developed to replace conventional alkali activators with engineered waste-derived silicate solutions synthesized from rice husk ash (RHA) and glass cullet. Comprehensive chemical, structural, and thermal characterization, including particle size analysis, X-Ray Fluorescence (XRF), X-Ray Diffraction (XRD), Field-Emission Scanning Electron Microscopy (FESEM), Fourier-Transform Infrared Spectroscopy (FTIR), and Thermogravimetric Analysis (TGA), was conducted to elucidate the influence of waste precursor chemistry on silica reactivity. Targeted pre-treatment routes, including controlled incineration and hydrothermal activation of RHA and alkali fusion of glass cullet following mechanical grinding, were optimized to enhance soluble silica yield and verified using Inductively Coupled Plasma (ICP) analysis. The resulting waste-derived silicate activators were employed in geopolymer binder systems, whose mechanical properties (compressive and flexural strength, setting time, and workability) and rheological behavior (viscosity, yield stress, and thixotropy) were systematically evaluated and benchmarked against conventional Na_2SiO_3-based systems. Comparable or superior performance was achieved in waste-derived geopolymer systems while offering significant reductions in embodied energy and carbon footprint, demonstrating a scalable and low-carbon pathway for valorizing agricultural and industrial wastes into high-performance geopolymer binders.

Keywords: Alkali Activators; Geopolymer; Silicate; Sustainable; Waste

Chemistry-informed e-waste recycling operations for informal recyclers targeting critical metals in the net-zero pathway

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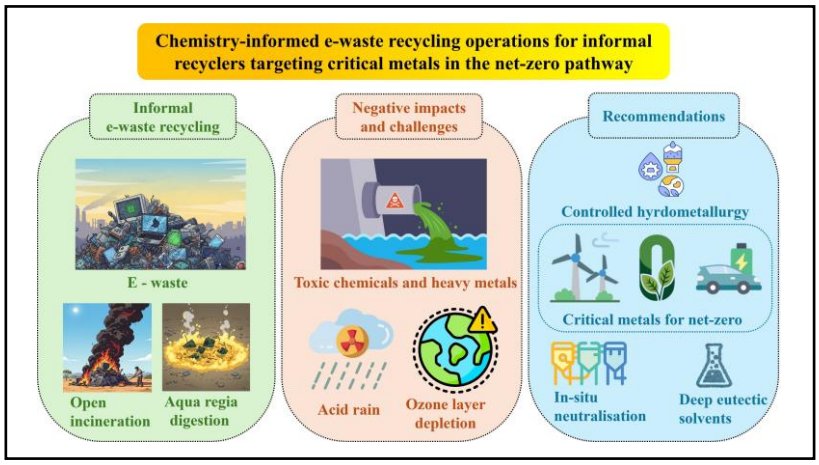
E-waste constitutes one of the most rapidly expanding waste categories worldwide. Developed countries manage e-waste through formal collection and recycling systems with environmental safeguards, while developing countries often lack such infrastructure and heavily depend on informal recyclers. Precious and base metals in e-waste, such as gold and copper, are extracted through aqua regia digestion and open incineration in informal recycling operations. These methods release hazardous chemicals and heavy metals into the environment, including them in the discarded waste streams. For example, the release of polychlorinated biphenyls poses severe environmental threats, contributing to acid rain and ozone depletion. The lack of gas-cleaning equipment allows harmful gases to be released into the atmosphere. Considering the potential of critical metal extraction from e-waste in our net-zero pathway, the transformation of informal recycling through chemistry-informed, sustainable metal-extraction operations is the way forward. Controlled hydrometallurgy techniques using mild acids or chelators, in-situ neutralisation of acidic waste, adsorptive filters for organics, and emerging green approaches, such as deep eutectic solvents, will allow for efficient metal leaching and recovery while addressing specific toxins. Given the socio-techno-economic constraints across developing countries, it is paramount to build capacity among informal recyclers for chemistry-informed e-waste recycling pathways yielding sustainability benefits.

Keywords: Chemistry-informed recycling, E-waste, Green chemistry, Informal recycling, Net-zero



Valorization of okara and okara-derived substrates through *Pleurotus ostreatus* mycelium biotransformation

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Soybean residue (okara) is an underutilized agro-industrial byproduct generated during soymilk and tofu production. As edible fungi can degrade a wide range of lignocellulosic biomaterials, fungal mycelium offers a promising approach for value addition to okara. Meanwhile, the development of alternative foods is increasingly important to meet future dietary demands. This study investigated the solid-state fermentation of 12 okara-based substrates using *Pleurotus ostreatus* mycelium and evaluated the potential of fermented okara as an alternative food. Dense mycelial growth was achieved within two weeks on fresh okara and wheat bran substrates. Fermentation significantly enhanced protein content, antioxidant capacity, and total phenolic content. Changes in non-volatile taste components, including soluble sugars, organic acids, free amino acids, and 5′-nucleotides, were also assessed. All substrates exhibited increases in glucose (178–539%), free amino acids (116–558%), and 5′-nucleotides (224–531%), while succinic acid became the dominant organic acid after fermentation. Electronic tongue analysis indicated reduced sourness and increased richness and umami taste, highlighting improved flavor characteristics. Overall, *P. ostreatus* demonstrated strong potential for the biotransformation of okara into nutritionally and sensorially enhanced food products.

Keywords: Waste valorization; solid-state fermentation; non-volatile taste components; alternative food; mycelium

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