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Day 1 September 23, 2024

ERATO Special Session - ROOM A

Challenges and Insight with Computational Heterogeneous Catalysis

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Heterogeneous catalysis of chemical reactions, including electrocatalysis, is widely applicable. However, it is a complicated process involving many factors that need to be considered including multiple phases, changes in conditions with time and electron transfer. Therefore, modelling these processes using computational methods is challenging. Despite this, computation studies offer the possibility to explore systems at the atomic level without perturbing the system which means that it has the potential to provide information that is inaccessible to experiment. Computational studies also enable unphysical situations to be created which can be valuable in elucidating the underlying cause of observed outcomes.

In this talk we will present some studies where we have used computational simulations to provide insight into catalytic processes[1-3] and other studies where our computational work has been combined with laboratory experiments to understand processes that are occurring.[4] Quantum chemical calculations using density functional theory and molecular dynamics simulations have been used in these studies that have led to development of models and information regarding the likely structures and dynamics.

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Nonmetal materials for catalytic reactions

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Highly reactive oxygen species (ROS), such as hydroxyl radical (•OH), sulfate radical ($SO_4^{\bullet-}$), high valent metals and singlet oxygen generated in advanced oxidation processes (AOPs), can degrade a wide array of organic contaminants. Therefore, continuous production of ROS by state-of-the-art strategies is highly favorable in water purification. However, these ROS with distinct redox capacity and reaction pathways display substrate-specific reactivity when reacting with organic pollutants. For traditional Fenton-like reactions, •OH suffers from high pH environment, self-quenching, solvent quenching, and scavenging by coexisting background organic/inorganic substances in real water matrixes (e.g., carbonates, halides, natural organic matters), which results in the diffusion-limited kinetics. In addition, the sluggish kinetics of Fe(III) reduction severely limit the long-lasting generation of ROS.

Currently, most of industrial catalysts are metal-based materials, which are both expensive and toxic to the environment. Recently, some inorganic materials have been employed for Fenton-like reactions for promoting ROS generation. Carbon is the richest element on the earth and can be employed as an alternative to metals as green catalysts. Here, I will present our research work on using nonmetal materials as catalysts and metal-free electron-sacrificers to promote ROS generation in Fenton-like reactions. We will discuss different materials in various reaction systems and their mechanism for ROS generation toward chemical synthesis and pollutant degradation.

Nanoparticle Platforms for Therapeutic Applications

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Advances in nanoparticle-mediated therapeutic delivery are poised to revolutionize disease treatment and prevention. In particular, the formulation of mRNA into lipid nanoparticles to combat COVID-19 has highlighted the transformative potential of nanoparticle platforms in the pharmaceutical industry and clinical practice. However, distinct types of therapeutics are required to meet specific therapeutic purposes and their encapsulation is typically tailored on a case-by-case basis. This presentation will present a versatile and biocompatible nanoparticle platform, whereby diverse therapeutics, including functional small molecules, siRNA, mRNA, and proteins, can be readily assembled into nanoparticles. The encapsulated therapeutics maintain their intrinsic activity and can be released upon exposure to the biological milieu. This nanoparticle platform has potential for usage in a range of applications.

Atom Transfer Radical Coupling: Harnessing ATRP for Organic Synthesis

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Controlling radical polymerization has been arguably one of the most important developments in polymer chemistry of the last few decades. The key processes, such as atom transfer radical polymerization (ATRP), nitroxide mediated polymerization (NMP) and reversible addition fragmentation chain transfer (RAFT) polymerization, were invented by taking established small molecule chemistry and using it in a novel way — to reversibly trap growing polymer radicals as dormant species so as to minimize termination. Since their inception, intensive research has led to massive improvements in polymerization control and scope through, for example the development of ATRP catalysts with increased activity, or the development of control agents that respond to alternative stimuli such as light, electricity or pH. These developments in turn offer new opportunities in small molecule synthesis. This presentation will outline one such opportunity: the use of ATRP catalysts to improve Cu-based cross-coupling techniques. We will outline a simple non-photochemical procedure for Cu(I)-catalyzed C–N coupling of aliphatic halides with amines and amides under mild conditions.[1] It uses Cu(I)Br, a commonly-used and inexpensive atom transfer radical polymerization (ATRP) precatalyst, along with the cheap ligand N,N,N',N",N"-pentamethyldiethylenetriamine (PMDETA), to activate the R–X bond of the substrate via inner-sphere electron transfer. The procedure brings about productive C–N bond formation between a range of alkyl halide substrates with heterocyclic aromatic amines and amides via a unique Cu(I)-Cu(II)-Cu(III)-Cu(I) cycle. As part of this talk, we will also describe our recent efforts to increase ATRP catalyst activity, with advantages for both polymerization and synthesis,[2,3] and how another ATRP-inspired strategy called ARGET-ATRP can be used to improve the air tolerance and selectivity of Cadiot−Chodkiewicz and Sonogashira couplings.[4]

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Single molecule nanotechnologies for applications in cancer and immunotherapy

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Modern medicine is currently transitioning to a new paradigm of precision and personalized care, where patients will be comprehensively screened and monitored for the detailed molecular abnormalities that characterise their specific disease. In the past decade, nanotechnology has provided new tools with unprecedented power to comprehensively interrogate genetic, transcriptomic and epigenetic information. The Centre for Personalised Nanomedicine at UQ is focused on translating these new technologies into a clinical setting, whilst simultaneously developing the next generation of point-of-care diagnostic and therapeutic technologies to further empower the personalised and precision medicine approach. As part of a major National Collaborative grant funded by the National Breast Cancer Foundation ("Enabling clinical epigenetic diagnostics: The next generation of personalized breast cancer care", CG-12-07), our consortium recently published hundreds of epigenetic regions that are highly informative in cancer, as well as a unique (and simple to detect) epigenetic marker that appears to be universal for cancer[1-3]. These are now being validated in a real-time clinical setting, where comprehensive DNA, methyl-DNA and RNA information is collected in tandem and analysed. In this talk we will present data on the clinical translation of this approach, highlighting some of the positive impacts that such an approach can make on the "recovery trajectory" of cancer patients. Along with comprehensive DNA/RNA/methylated-DNA sequencing methodologies, several point-of-care nanotechnologies recently developed by our lab will be presented.[e.g.,4-8]. These include novel technologies for detecting circulating free DNA/RNA/methyl-DNA, circulated tumour cells, exosomes and protein biomarkers, as well as single-molecule read-out systems to monitor the immune system in real time.

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Boron Nitride Nanotubes and Nanosheets: Synthesis, Properties and Applications

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Synthetic routes and electromechanical properties of pristine and carbon-doped BN nanotubes[1] and graphene-like nanosheets, so called “boronitrines”, are investigated. Access to properties was achieved through employing state-of-the-art methods of *in situ* and *operando* high-resolution transmission electron microscopy (TEM).[2] Elastic modulus, tensile strength,[3,4] fracture toughness, conductivity of 1D and 2D BN-based nanostructures are measured in different morphologies, dimensions and defectiveness of the samples. Various modern *in situ* holders allowing for current-voltage and/or force-displacement curve measurements and shining light of various wavelengths onto the nanostructures are utilized in high-resolution electron microscope columns under atomic resolution. Based on the TEM results, emerging practical applications of BN-nanomaterials as effective supports for most common catalytic reactions, *e.g.*, CO_2 hydrogenation, CO oxidation *etc*., hydrogen accumulation,[5] secondary-ion batteries, reinforcing agents in light metals and polymers, and water purifiers are also shown. The results are supported by first-principle theoretical calculations.

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Materials Innovation for Green Hydrogen Production and High-performance Batteries

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Global warming and climate change are the biggest challenge facing humanity in the 21st century. My centre mainly focuses on developing efficient energy devices for sustainable energy production, storage, and conversion.

In this talk, I will briefly introduce my team's achievements in several key sustainable energy technologies through rational materials design and innovative materials synthesis. These include (i) Electrochemical catalysts for green hydrogen production[1,2]. Single-atom catalysts offer a pathway to cost-efficient catalysis with the minimal amount of precious metal used but creating them and keeping them stable during operation is a challenge. Double transition-metal MXene nanosheets, $Mo_2TiC_2T_x$ were fabricated with abundant exposed basal planes and Mo vacancies in the outer layers by electrochemical exfoliation. The developed catalyst exhibits an outstanding catalytic ability with a low overpotential and a mass activity about 40 times greater than the commercial platinum-on-carbon catalyst; (ii) Lithium-ion and lithium-air batteries for electrification of road transport such as electric vehicles[3-5]. I will report on a recent development on an ionic liquid bearing the redox active 2,2,6,6-tetramethyl-1-piperidinyloxy moiety, which serves multiple functions as a redox mediator, oxygen shuttle, lithium anode protector, as well as electrolyte solvent. The additive contributes a 33-fold increase of the discharge capacity in comparison to a pure ether-based electrolyte; (iii) Low-cost rechargeable batteries for grid-scale renewable energy[6,7]. Sodium-based batteries are being considered as a promising system for low-cost stationary energy storage and conversion, owing to the natural abundance of sodium. Several electrode materials and electrolytes were synthesized for sodium metal batteries and sodium-sulfur batteries; (iv) Rational design of electrolyte systems for improving the safety of high-energy batteries[8,9]; and (v) Facile and sustainable recycling of spend lithium-ion batteries[10].

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Day 2 September 24, 2024

ERATO Special Session - ROOM A

ERATO Overview: Towards the 2nd generation of porous materials

Yusuke Yamauchi, The University of Queensland, Australia
Nagoya University, Japan

In the ERATO project, we aim to create novel inorganic nanosolids with internal nanospaces, representing unprecedented nanospace materials. We will develop methodologies for their effective integration to exploit the functions derived from the synergistic fusion of various supramolecular, photonic, and magnetic behaviors occurring within these nanospaces. Our research will cover a wide range of porous systems, including metals, carbons, sulfides, phosphides, and transition metal oxides. Additionally, we will efficiently integrate machine learning with our inorganic synthesis methods to accelerate the optimization of synthetic parameters for the design of target materials and to identify optimal combinations of inorganic blocks for material integration.

Flexible mesopores in nanoscrolls: Extraordinarily large alteration of pore sizes and their reversibility

Yusuke Asakura, Nagoya University, Japan

Nanoscrolls, a unique form of nanomaterials characterized by their rolled-up nanosheet structures, offer significant potential as flexible mesoporous materials due to their tunable pore sizes and structural versatility. In this study, we demonstrate the reversible and extraordinarily large alteration of pore sizes within niobate-based nanoscrolls through a series of ion exchange reactions. By intercalating different cations into the interlayer spaces of nanoscrolls, we achieve significant control over the size of the inner one-dimensional mesopores, a property that sets these materials apart from previously reported flexible porous materials.

We synthesized niobate nanoscrolls containing dodecylammonium ($C12^+$) cations and dioctadecyldimethyl ammonium ($C18_2Me_2^+$) cations through the reaction of protonated layered hexaniobate with dodecylammonium chloride and dioctadecyldimethylammonium bromide, facilitated by the pre-intercalation of tetrabutylammonium cations. The resulting nanoscrolls exhibited significant structural flexibility, as evidenced by large alterations in pore size when subjected to ion exchange treatments with NH_4Cl ethanol solution. Notably, $C12^+$ cations showed an extraordinarily large pore size alteration, expanding from approximately 10 nm to over 20 nm, which is a significant increase compared to the alterations observed in other flexible porous materials like metal-organic frameworks (MOFs) and porous carbons.

Our study further explores the reversibility of these pore size alterations by re-inserting bulky cations into the interlayer spaces. TEM and SEM analyses confirmed that the nanoscrolls maintained their structural integrity throughout these modifications, with pore sizes returning to their original dimensions upon re-intercalation of the original cations. This reversible behavior underscores the potential of nanoscrolls as host materials for stimuli-responsive applications.

In summary, this study presents niobate nanoscrolls as a promising class of flexible mesoporous materials with an unparalleled ability to undergo reversible and significant alterations in pore size. The insights gained from this research not only enhance our understanding of nanoscroll behavior but also open up new possibilities for their application in various technological fields, where control over pore structure and electronic properties is essential. The reversible and large-scale alteration of pore sizes, combined with the potential for bandgap tuning, positions nanoscrolls as a versatile and valuable material in the advancement of nanotechnology.

Giant piezoresponse in nanoporous (Ba,Ca)(Ti,Zr)O_3 thin film

Md. Shahriar A. Hossain, The University of Queensland, Australia

The effects of lattice strain on the piezoelectric properties of crystalline ferroelectrics have been extensively studied for decades; however, the strain dependence of piezoelectric properties at the nanoscale has yet to be thoroughly investigated. Herein, we report, for the first time, a new perspective on the super-strain of nanoporous polycrystalline ferroelectrics using a nanoengineered barium calcium zirconium titanate composition, $(Ba_{0.85}Ca_{0.15})(Ti_{0.9}Z_{0.1})O_3$ (BCZT). Atomic-level investigations reveal that controlled pore wall thickness contributes to highly strained lattice structures while maintaining crystal size at an optimal value (<30 nm), which is a key factor in achieving high piezoelectricity. The strain field, derived from geometric phase analysis at the atomic level and aberration-corrected high-resolution scanning transmission electron microscopy (STEM), yields over 30% and shows strong theoretical agreement with high piezoelectric properties. The uniqueness of this work lies in the simplicity of the synthesis, and the resulting piezoresponse d_{33} becomes exceptionally large, around 7500 pm V^{-1}. This response is an order of magnitude greater than that of lead zirconate titanate (PZT), which has been the most successful ferroelectric over the past 50 years. This nanoporous BCZT concept holds great promise for developing high-density, electrolyte-free dielectric capacitors and generators for energy harvesting in the future. In this presentation, additional examples of nanoporous materials will be presented

Significant impact of interfacial controls in nanomaterials

Miharu Eguchi, Waseda University, Shinjuku, Tokyo, Japan

To increase chemical reaction rates, common strategies include raising the concentration or temperature and introducing catalysts. In this study, we accelerated the rate constant of an electrophilic metal coordination reaction by 23-fold on the surface of layered aluminosilicate (LAS). This enhancement occurs because the reaction substrate (ligand molecule) induces dielectric polarization on the polar and anionic LAS surface. According to the Arrhenius plot, the frequency factor (A) increased by nearly three orders of magnitude on the surface, suggesting that the collision efficiency between ligands and metal ions is enhanced due to dielectric polarization. This finding is unexpected, as one side of the ligand is obscured by the surface, which would typically reduce collision efficiency. This novel method for accelerating chemical reactions may broaden the applications of LASs, which are chemically inert, abundant, and environmentally friendly. The concept is also applicable to other metal oxides with polar surfaces, potentially benefiting a variety of chemical reactions in the future. In this presentation, additional ongoing topics, including high-entropy alloys and interfacial controls, will also be discussed.

Enabling more deterministic SERS sensing of environmental contaminants using hierarchical porous metals

Joel Henzie, National Institute for Materials Science (NIMS), Japan

Low-cost detection systems are needed for the identification of toxic chemicals in environmental samples. However, their rapid identification is hindered by the need for complex isolation and pre-treatment methods. We will describe a comprehensive sensing platform to identify MPs in environmental samples without requiring independent separation or pre-treatment protocols. It leverages the physicochemical properties of macroporous-mesoporous silver (Ag) substrates templated with self-assembled polymeric micelles to concurrently separate and analyze multiple MP targets using surface-enhanced Raman spectroscopy (SERS). The hydrophobic layer on Ag aids in stabilizing the nanostructures in the environment and mitigates biofouling. To monitor complex samples with multiple MPs and to demultiplex numerous overlapping patterns, we develop a neural network (NN) algorithm called SpecATNet that employs a self-attention mechanism to resolve the complex dependencies and patterns in SERS data to identify six common types of MPs: polystyrene, polyethylene, polymethylmethacrylate, polytetrafluoroethylene, nylon, and polyethylene terephthalate. The combination of macroporous-mesoporous substrates, organic surface agents, and self-attention-based NN technology holds the potential to enable MPs to be field monitored by generating rich datasets that machines can interpret and analyze.

In-situ self-assembled nanomolecular systems for selective sensing applications

Jonathan P. Hill, National Institute for Materials Science, Japan

Modulation of the properties of organic chromophores is made possible by their incorporation in aggregated structures, and so it has become an extremely active research area. Supramolecular chemistry and self-assembly methods are key means to influence aggregative processes, and can be used to control the emergent properties of self-assembled organic nanomaterials. Porphyrins and other tetrapyrrole chromophores are highly suitable for sensing operations based on their synthetic flexibility and molecular structures where an analyte might interact to stimulate some variation in directly observable optical color or fluorescence emission modulation. However, a more technologically viable means of accessing the sensing responses of these compounds is required in order to integrate the sensing properties of the porphyrins especially with solid-state devices. In this work, we have achieved this by the physical interfacing of a synthetic supramolecular material with a membrane-type surface stress sensor (MSS). Deposition by self-assembly from solution of a family of special porphyrin derivatives (NiOxx) establishes a hierarchically porous nanocrystalline network of the molecules on the MSS substrate, which enables a direct detection of the sensing responses caused by introduction of an analyte to the self-assembled material. The resulting self-assembly-MSS device is portable and can be used to detect target analytes even under conditions of high humidity. Remarkably, the molecular structure of the NiOxx derivative strongly affects the sensing selectivity of the device demonstrating that molecular level interactions can be amplified to a level detectable using the membrane-type sensor. Subtle variations in the molecular structure can be used to tune the sensing properties towards different analytes so that the MSS-NiOxx can be used in a wide variety of sensing scenarios such as diabetes monitoring (acetone sensing), bioreactor monitoring (volatile fatty acid differentiation), and other difficult to achieve sensing operations. Different aspects of the systems including structural and mechanical features of MSS-NiOxx devices will be discussed. X-ray crystal structures of the self-assembled chromophore materials will be presented. Properties of some other porous porphyrin materials will be mentioned.

Synthesis of chiral Au nanostructures on mesoporous Au substrates for enhanced chiral sensing applications

Kenta Nakagawa, Waseda University, Japan

“Chirality” is a property of three-dimensional object or phenomenon that cannot be superimposed on its mirror image by any combination of translations, rotations, and reflections. Chirality appears in many molecules, crystals, and nano-structures and is also important for understanding not only the structures of chemical substances but also the functionalities of life. Since chirality of our body is biased (e.g., we are made from only L-from of amino acids and D-form of sugars, respectively), our body responds differently to each chiral isomers (enantiomers). When the chiral substance is pharmaceuticals or pesticides, pharmacological difference between the enantiomers is appeared as medicinal positive effects and negative toxicity. Therefore, it is very important to develop the methods or devices that enable us to discriminate the enantiomers easily and precisely.

Because chiral molecules exhibit a polarization-dependent interaction with light, optical analytical techniques such as circular dichroism (CD) spectrophotometer and polarimeter are well suited to sense and characterize chirality. CD spectroscopy senses the difference of absorption between left- and right-circularly polarized light and polarimeter senses the rotation of the plane of incident linearly polarized light originated from the difference of refractive index between left- and right-circularly polarized light. As circularly polarized light itself is chiral, the difference of absorption and/or refractive index between left- and right- circularly polarized light is occurred due to the interaction between chiral circularly polarized light and chiral molecules. However, the interaction is inherently weak because the size of molecules we focus on are about 10^3-10^5 times smaller than the wavelength of circularly polarized light they are sensed with, resulting in small signals on the order of millidegrees. Thus, large quantities of samples are required for adequate signal-to-noise ratios. In contrast, metallic nano structures such as nano particles, nano rods, or mesoporous structures exhibit an especially strong optical response due to their localized surface plasmon resonance, which is the coherent oscillation of free electrons in the metals upon exposure to an oscillating electromagnetic field. The optical response of the nanostructures depends on its size, shape, and chemical composition, all of which can be controlled with optimized chemical synthesis. Therefore, control of nanostructure is a quite important issue in materials chemistry to bring out unique optical response.

In this study, we developed a hierarchical nanostructure of chiral Au nanostructures on mesoporous Au substrates by only electrochemical techniques. By considering the chemistry of the electrolyte solution, we successfully achieved control of the morphology of the Au nanostructures, which exhibit CD. In addition, by measuring the SERS spectra from several types of amino acids analytes on the mesoporous chiral Au, we discuss the potential and the detection mechanism for the analysis of chiral molecules by using the films.

Session: Ceramics, Polymers and Composite Materials

Liquid Metal-Polymer Composites: A Soft-Soft Combination with Exciting Properties

Shiyang Tang, The University of New South Wales, Australia

Crack healing for robust environmental barrier coating

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SiC fiber-reinforced SiC matrix composites (SiC_f/SiC_m) are being evaluated as potential materials for next-generation gas turbine blades. However, SiC exhibits susceptibility to volatilization and recession in high-temperature water vapor rich environments. This vulnerability necessitates the application of environmental barrier coating (EBC). Among candidate EBC materials, β-$RE_2Si_2O_7$ have emerged as promising options due to their chemical stability and thermal expansion coefficient compatibility with SiC. Conventional thermal spraying processes used for coating deposition often produce amorphous phases with residual cracks and pores which compromises EBC effectiveness. Recent studies have explored incorporating carbide particles (e.g. SiC or TiC) into structural materials to facilitate crack healing through oxidation-induced volume expansion. Most studies have examined crack healing behavior in ambient air. However actual harsh environments contain water vapor. Therefore elucidation of crack healing behavior in various environments including high-temperature water vapor-rich conditions is important.

This study aims to elucidate the crack healing mechanism in β-$Yb_2Si_2O_7$/SiC composites, a leading EBC material candidate. $Yb_2Si_2O_7$ composites containing 5 vol% or 10 vol% dispersed SiC were fabricated via solid-state reaction and hot-press sintering at 1550℃ for 1 h in Ar under 30 MPa. Characterization was carried out using field emission scanning electron microscopy (FE-SEM), field emission electron probe microanalysis (FE-EPMA), and X-ray diffraction (XRD). Cracks were introduced using Vickers indentation, followed by annealing in air or water vapor rich environments at temperatures ranging from 750°C to 1400°C for durations up to 50 h.

The introduction of cracks in the samples reduced their flexural strength. Following air annealing, both samples exhibited decreased crack length and increased flexural strength correlated with rising temperature. Notably, the strength exceeded initial values after exposure at 850 °C for 1 h, even in the absence of complete crack healing. Post-annealing fracture toughness increased, indicating that oxidation-induced compressive stresses significantly contributed to strength recovery. On the other hand, crack healing was enhanced in a water vapor-rich atmosphere. This enhancement is attributed to the accelerated diffusion of H_2O into SiO_2 compared to O_2. In atmospheres with high water vapor partial pressure, H_2O diffusion through the SiO_2 layer formed on SiC particles promotes oxidation of the underlying SiC. Exposure at 1400 °C for 50 h in air resulted in no significant exfoliation. However, in water vapor-rich environments, excessive SiC oxidation can induce intolerable compressive stresses, leading to delamination. In high-temperature water vapor environments, $Yb_2Si_2O_7$ decomposes to Yb_2SiO_5 and subsequently reacts with SiO_2 (an oxidation product of SiC) to regenerate $Yb_2Si_2O_7$. This reaction results in volume contraction, potentially suppress excess volume expansion of SiC and mitigating excessive stresses.

These findings indicate that appropriate SiC incorporation can effectively induce crack filling, enhance mechanical properties, and extend EBC lifetimes through a self-healing mechanism in both air and water vapor-rich environments.

Robust Structures from Natural Plants

Binodhya Wijerathne, Queensland University of Technology, Australia

DAY – 2 24 September, 2024- Room B

Session: Energy and Environmental Materials

Generating Green Hydrogen from 2D Materials

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Next-Generation Sulfur Cathode:

Electrocatalyst to Accelerate Sulfur Conversion Reaction

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Although lithium-sulfur (Li-S) batteries have been expected as a promising high-energy-density battery system, entangled problems in each cell component hamper their practical use. Especially in cathode, low electronic/ionic conductivity of sulfur based active material, continuous dissolution of polysulfide, and sluggish redox kinetics cause the poor cycle stability and energy density. For the energy density of 500~600 W h kg^{-1}, achievement of high areal sulfur loading and low electrolyte to sulfur (E/S) ratio is needed, but conventional carbon/sulfur composite-type cathodes have limitations to satisfy this requirement. In this seminar, next-generation sulfur cathode with the electrocatalyst accelerating the sulfur conversion reaction is introduced as a powerful platform to simultaneously improve the cycle stability, reversible capacity, and rate capability. This seminar aims to present comprehensive overview of previously conducted studies and future research direction to design the efficient electrocatalyst for sulfur cathode. In particular, strategies to search for new electrocatalyst, to improve the catalytic activity and stability of catalyst, and to fundamentally understand the electrocatalytic trends in sulfur cathode will be covered. We believe development of optimized catalytic materials in cathode with the deep fundamental understanding on electrocatalysis enables realization of high areal sulfur loading and low E/S ratio for high energy density of Li-S batteries.

Biography

Jinwoo Lee obtained his B.S. (1998) and Ph.D. (2003) degrees from the Department of Chemical and Biological Engineering of Seoul National University (SNU), Korea. After postdoctoral research at SNU (with Prof. Taeghwan Hyeon) and Cornell Univer-sity (with Prof. Ulrich Wiesner), he joined the faculty of the Department of Chemical Engineering at POSTECH (2008–2018). In 2018, he joined the faculty of the Department of Chemical and Biomolecular Engineering at KAIST. His researches focus on synthesis and applications of designed nano-functional materials for energy conversion and storage devices.

Advanced Atomic Catalysts Design for Energy Systems

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Semiconductor catalyst-based composite systems for environmental betterments:
a case of photo-hydrogenation of CO_2 to methanol

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The attention on environmental science is for greenhouse gas, microplastics, water pollutants, etc. Especially, the emission of CO_2 gas, which is a majority among greenhouse gases, has been first on the serious environmental issues due to its continuous growth within atmosphere as a consequence of remarkable rapid growth in global consumption of carbon-based energy. On the other hand, the breaking in the renewable energy technology is also the important issue from the view point of restraining the emission of CO_2 and the exhaust of biofuels. Thus, converting CO_2 to fuels is a promising solution to environmental and energy issues. In this talk, we report the CO_2-to-methnol hydrogenation reaction using semiconductive metal oxide hybrid catalysts, which are synthesized by the physical bottom-up synthesis procedure and provided the catalyst scaffold and the CO_2 adsorber. Although the photodegradation of CO_2 produce different molecules like CH_4, CO, methanol, aldehyde, and formic acid, CH_4 and methanol are raw materials of fuels. CuO and ZnO can selectively produce methanol, but their hybrid enhances the photoreaction. On the comparison of the nanoparticle-nanoparticle, nanoparticle-cluster and cluster-cluster combinations of CuO-ZnO hybrid particles, the nanoparticle-nanoparticle hybrid contributes to the photoreaction involving the heterojunction formation but the cluster-cluster hybrid is followed on the reacting surface area increase involving the size decrease. The systems consisting of catalysts alone is still not enough for high performance of the photoreaction of CO_2. One of reason should be the less possibility for CO_2 gas to reach on the active surface of catalysts. Thus, the introduction of the CO_2 binding sites was performed in the catalytic systems. The effective binding site is the anime group, which is included in molecules like poly(amido amine) dendrimer, chitosan and 3-amino-propyltriethoxysilane. Another designing is the utilization of scaffold like metal-organic frameworks, where semiconductive particles are deposited in/on the scaffold. The additional upgrade is the enlargement of the reactive surface area per volume. It is solved using 3-dimensional substrate, and then the reaction surface increases 1.2 times. After these developments of the catalytic systems, the photo-hydrogenation succeeded the two-order enhancement of the reaction. In addition, the presented film-type catalytic system is convenient for the separation of catalyst systems from the product and the reaction system.

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Scanning probe microscopy imaging of line defect on rutile TiO_2(110)-(1×2)

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TiO_2 is one of the famous photocatalysts applied for various fields such as water splitting catalysts, coating materials, and solar cells. The reaction field of photocatalyst is the surface. For obtaining the design guidelines of high reactive photocatalysts, it is important to understand the surface structure and the elementary process of photocatalytic reaction as the reaction field.

Rutile TiO_2(110) surface have been used as a model surface for the study of a photocatalyst. The rutile TiO_2(110)-(1×1) surface transforms to the (1×2) surface by iterations of Ar^+ sputtering and high-temperature annealing over 900 °C. The (1×2) surface structure is an asymmetric periodic row structure. The (1×2) surface has various local structures: the single-link structure, the double-link structure, and the line defect. Among these local structures, the line defect has been reported with no reactivity of water adsorption [1]. The origin of no reactivity of water adsorption is still controversial. In this study, we investigated the line defect on rutile TiO_2(110)-(1×2) surface using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM).

Nb-doped (0.05 wt%) rutile TiO_2(110) substrates (Shinkosha) were used for the sample. The (1×2) surface was prepared by iterations of Ar^+ sputtering (Ar partial pressure: 2.5×10^{-4} Pa, Energy: 1.5 keV) and annealing at 1000 °C under the ultra-high vacuum ($< 5.0 \times 10^{-8}$ Pa).

In the case of NC-AFM imaging of metal oxide surfaces, the contrast of NC-AFM image depends on the tip apex polarity [2]. We obtained NC-AFM image of the line defect with opposite contrast to each other. This result suggests that the line defect has charge polarity. To confirm this assumption, the contact potential difference (CPD) on line defects and (1×2) periodic rows were evaluated using NC-AFM. The comparison of the CPD between line defects and (1×2) periodic rows reveals that the line defects were charged relatively negative from (1×2) periodic rows. Furthermore, atomic-resolution NC-AFM image was obtained to elucidate the line defect structure. The atomic-resolution NC-AFM imaging unveiled the structure of the line defect.

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Promotion effect of W^{6+} and Ga^{3+} cations on the photocatalytic activity of $Zn^{2+}Al^{3+}$ layered double hydroxides (HDLs) and ZnAl mixed oxides obtained from their $Zn^{2+}Al^{3+}$ LDHs in the photodegradation of contaminants diclofenac and 4-chlorophenol in aqueous medium.

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The photocatalytic activity of ZnAlW-*x* layered double hydroxides (where $x = 1.5$, 3.0 and 5.0 mol% of W^{6+} cations) prepared by coprecipitation was studied in the photo-degradation of diclofenac in aqueous medium using UV light irradiation. The incorporation of W^{6+} cations within the ZnAl layered double hydroxide brucite- type layer structure promoted the decrease in the band gap energy and the inhibition in the recombination rate of electron-hole pairs as well as the improvement in photocatalytic activity in the degradation of diclofenac in aqueous medium. Such improvement in the photocatalytic activity could be favored by the increase in the positive charge of the ZnAl layered double hydroxide sheets due to the incorporation of W^{6+} cations. ZnAl layered double hydroxide photodegaradate 29.0 % of diclofenac at 90 min of photoreaction. However, the photodegradation % of diclofenac increased with the molar concentration of W^{6+} to achieve 68.0% in 40 min and 82.0 % in 90 min of photoreaction respectively using ZnAlW-1.5 or ZnAlW-3 layered double hydroxides. The kinetics studies and total organic carbon analysis confirmed the highest efficacy of ZnAlW-1.5 and ZnAlW-3 layered double hydroxides to photodegradate and mineralize diclofenac molecules in aqueous medium. On the other hand, the photocatalytic activity of ZnAlGa-*x* ($x = 0$, 0.5, 0.8, 1.0, 2.0 and 3.0 mol % of Ga^{3+}) mixed oxides obtained by calcination from their corresponding layered double hydroxides was studied in the photodegradation of 4-chlorophenol in aqueous medium using UV light irradiation. Structural studies by X-ray diffraction, Raman and EPR spectroscopies of ZnAlGa-*x* mixed oxides indicated that the incorporation of a small molar concentration of Ga^{3+} cations (0.5–0.8 mol %) within the ZnAl layered double hydroxides structure changed their crystalline structure to an amorphous structure and promoted the formation of a high amount of structural oxygen vacancies. Transient photocurrent response and fluorescence spectroscopy results revealed that the incorporation of a small molar content of Ga^{3+} in the structure of ZnAl mixed oxide promoted the enhancement in the transient photocurrent response, the separation of photogenerated charges and the inhibition of the recombination rate of electron - hole pairs. Moreover, ZnAlGa-*x* mixed oxides with a small molar concentration of Ga^{3+} reduced their band gap energies below of 3.0 eV. ZnAl mixed oxide photodegradated 69.0 % of 4-chlorophenol at 4 h of photoreaction. However, the photodegradation % of 4-chlorophenol increased to 80–90 % with approximately 70-75 % of mineralized dissolved total organic carbon at 3 h of photoreaction using ZnAlGa-*x* mixed oxides with a small molar concentration of Ga^{3+}. The photocatalytic degradation reaction of 4-chlorophenol fitted well to a pseudo-first order kinetics of Langmuir-Hinshelwood-type. The kinetic studies of ZnAlGa-*x* mixed oxides confirmed that ZnAlGa-0.8 mixed oxide was the best photocatalyst to photodegradate 4-chlorophenol in aqueous medium. The highest photocatalytic activity and efficacy of ZnAlGa-0.8 mixed oxide to mineralize 4-chlorophenol in aqueous medium may be due to its higher amount of oxygen vacancies generated in its structure promoting a better separation of charges and the inhibition in the recombination rate of photogenerated electron – hole pairs.

Heterogeneous transition metal-based electrocatalysts for water splitting and CO_2 reduction

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A several of crises such as energy shortage, global warming, and air pollution are occurred by the utilization of fossil fuels, thus it fascinates the researchers to advancement of environmentally friendly, and sustainable substitute energy sources. The hydrogen (H_2) molecule is a promising type of fuel having energy density (33.6 kWh per kg) which is higher than diesel and gasoline. Overall water splitting generates H_2 and O_2 from water via the hydrogen evolution reaction (HER) at the cathode and oxygen evolution reaction (OER) at the anode. This energy conversion method has attracted attention due to its negligible production of pollution, various applications, and astronomical energy conversion efficiency[1, 2]. The overall water splitting required highly active electrocatalysts to facilitate both HER and OER reactions. For HER, Pt group metals are highly effective as electrocatalysts. And for OER, benchmark electrocatalysts are Ir/Ru-based materials. However, high cost and rarity of these metals limits their pragmatic use. Currently, enormous effort has been taken to the advancement of transition metal based electrocatalysts due to their low cast and abundant in nature[1, 2]. There are variety of transition metal based electrocatalysts have been investigated as bifunctional electrocatalysts (for HER and OER) for overall water splitting such as alloys, oxides, chalcogenides, phosphides, carbides, phosphate, and hydroxides[1, 2].

The anthropogenic carbon dioxide (CO_2) is a major responsible to the global warming. The current industries such as cement and steel industries which produces about 8% and 5% of the global level CO_2 emissions. The goal of research communities is to get net-zero emissions will be achieved by carbon recycling. The electrochemical conversion CO_2 reduction reaction (ECO_2RR) powered by renewable sources is a smart sustainable substitute to the fossil resources[3]. The ECO_2RR may undergo various multi-electron-proton pathways, resulting to a wide range of carbon-based chemical products. In ECO_2RR, selectivity is a major challenge since competitive with undesired ECO_2RR mechanisms and HER may obstruct the generation of a specific product. The CO_2 molecule is very stable and extreme inertness in nature which lead to both kinetic and thermodynamic restriction for an efficient ECO_2RR. A transition metal-based catalysts are useful to lower the above-mentioned barrier and drive the ECO_2RR process at acceptable potentials and rates. The interaction of the electrocatalytic metal center with ECO_2RR intermediates is required to determine the selectivity of specific product[3]. In the last decades, a variety of transition metal-based electrocatalysts have been investigated for efficient ECO_2RR, varying from molecular electrocatalysts to metal nanoparticles and heterogeneous nanomaterials. There are still have opportunity to improve electrocatalyst performances in terms of selectivity, activity, and stability for pragmatic applications[3].

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Single-atom catalysts for energy storage and conversion

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Efforts toward developing clean and sustainable electrochemical energy storage and conversion have garnered significant interest. Overcoming the challenges of creating next-generation systems with enhanced activity and prolonged cycling stability remains a significant endeavor. Numerous catalysts have been investigated to enhance electrochemical reactions. Within the spectrum of explored catalysts, single-atom catalysts (SACs) have emerged as particularly noteworthy their maximum atom utilization efficiency, exceptional electronic structure, homogeneous active centers, and unsaturated coordination environment.[1-2] In this abstract, the recent advances of the synthesis methods for SACs and the recent progress of SACs for energy storage and conversion, including lithium selenium batteries, lithium-ion batteries and zinc air batteries will be presented. 1) We developed a facile route to synthesize cobalt single atoms/nitrogen-doped hollow porous carbon. The cobalt single atoms can activate selenium reactivity and immobilize selenium and polyselenides. The as-prepared selenium-carbon cathodes deliver a high discharge capacity, a superior rate capability, and excellent cycling stability with a Coulombic efficiency of ~100%.[3] 2) We have synthesized hollow-structured SiO_x@carbon nanotubes (CNTs)/C architectures with graphitic carbon coatings and in situ growth of CNTs. When applied as anodes in LIBs, the SiOx@CNTs/C anodes exhibit high reversible capacity, high initial Coulombic efficiency (88%), outstanding cycling performance, and extraordinary mechanical strength during the calendaring process (200 MPa).[4] 3) We rationally designed and synthesized a series of transition metal-nitrogen-carbon (TM-N-C) SACs for ORR, which are also identified using computational screening. Remarkably, the as-prepared FeH-N-C SACs with an ultra-low Fe loading of 0.2 wt% exhibited outstanding endurance, which can undergo 100,000 voltage cycles with low half-wave potential loss and no apparent structure changes.[5] In addition, Fe-N-C SACs also present a long-term stability over 1200 h in rechargeable zinc-air batteries.

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Metal-Support Interaction in Catalysis

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Enhancement of Electrocatalytic Activity of Metal-Organic Frameworks for Water Splitting at Elevating Temperatures

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Accelerating Materials Discovery Through High Throughput Simulations

and Machine Learning Approach for Energy and Environmental Applications

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High-Performance Semitransparent Organic Solar Cells and Modules

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Thin-film solar cells made with polymer and perovskite absorbers represent a transformative technology with great potentials for high-throughput manufacturing at very low cost. In this talk, we will discuss the integrative approach to access high-performance polymer and perovskite solar cells, including the results of champion organic solar minimodules made in lab that have been published in the "Solar Cell Efficiency Table" by Prof. Martin Green (59th, 60th, 61st and 62nd editions), as well as our efforts in fabricating inverted perovskite solar cells with the certified efficiency over 26%.

Specific emphasis will be placed on our efforts on pilot production of large area see-through photovoltaics via a new design of semitransparent organic solar cells and modules, which allows for the efficient utilization of spectrum-engineered solar photons from the visible to infrared range with both energy generation and saving features. Model analysis indicated that the installation of these see-through power windows worldwide would contribute to the carbon neutrality of society.

KEYWORDS

n-Doping, Interfacial layer, Solar cell, Semitransparent

Dynamically Engineering Nanostructured Electrodes for Advanced Electrochemical Devices

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With the presence of multi-physics fields the evolution of nanostructures and the electrochemical process can undergo complicated processes, which have been making it particularly difficult to control. The classical Self-organization Theory says that a proper energy and informational flow can trigger local interactions between elements in a system and thus incur emergence of regular patterns with resilience and adaptation characteristics. But for many electrochemical devices, exploring novel methods to conform/regulate reversible electrochemical reactions and maximize mass transfer efficiency has been challenging and yet to be explored. In this talk, the speaker will introduce a series of intriguing self-evolving cases of new-concept electrochemical devices including batteries, electrolyzers and electrochromic windows, and the how some of the techniques are being transferred[1-6]. He will showcase some recent progresses on manipulating bubbling behavior of anisotropic metallic aerogel for upgraded water splitting at extremely high current densities, engineering safer battery anodes by regulating the dendrite evolution patterns, and a conceptual electrochromic window based on dual-dissolution/deposition electrode reactions for unprecedented performance.

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Towards Bio-Inspired Hydrophobic Modifiers for the Treatment of Clay Minerals

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Mineral processing is a world-wide industry that provides precious metals and other elements for use in technologies that are crucial for solving our energy and environmental challenges. The treatment of slime water in mineral processing is critical for maintaining the quality of circulating water and downstream industrial processes. Phyllosilicate minerals, particularly clay minerals such as kaolinite, montmorillonite, and illite, are common in mineral tailings, posing challenges to dewatering due to their fine granularity and surface properties. Of these minerals, kaolinite is prevalent in various mineral tailings, including those from coal preparation and oil sands processing plants.

This study is aimed at designing and synthesizing novel bio-based molecules, inspired by naturally occurring substances to address the drawbacks associated with synthetic polymeric and small molecular surfactants/flocculants commonly employed in the dewatering process. These novel molecules hold promise for enhancing the turbidity removal and settling efficiency of fine kaolinite (10µm) particles through hydrophobic agglomeration.

Several bio-inspired surfactants were synthesized by modifying a naturally occurring molecular framework incorporating amine functionality to enhance surfactant-clay interactions alongside the installation of hydrophobic moieties to modulate the surfactant properties. UV/Vis spectroscopy measurements of supernatants, diffuse reflectance, Fourier transform infrared spectroscopy, and powder X-ray diffraction measurements were performed to gain insight into the surface adsorption on kaolinite. Potential interactions between the surfactant and the kaolinite surface were proposed by employing spectroscopic measurements and single crystal structure analysis which provided insights into the molecular configuration of the surfactants. The impact of these surfactants on the surface hydrophobicity of kaolinite was evaluated using the Washburn capillary rise method. Notably, treatment of kaolinite with 0.05% wt. of the best performing surfactant resulted in an improvement of the contact angle from 66.8° to 82°. Aggregate size measurements following surfactant dosing under stirring conditions were conducted using an image-derived particle size measuring technique, the impact of which on surface hydrophobicity and particle size was systematically evaluated. Gravitational sedimentation under non-stirring conditions and turbidity removal efficiency of the supernatants of surfactant treated kaolinite slurries were also examined. Overall, the study demonstrates that our surfactants significantly enhance the settling and clarification of kaolinite slurries, offering a promising, environmentally sustainable alternative to traditional synthetic surfactants in mineral processing applications.

Multilayered Graphene Membrane for Flexible Ammonium-ion Storage Device

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Ammonium-ion (NH^{4+}) energy storage systems offer a promising path for large-scale, inherently safer energy storage solutions. Unlike their metallic counterparts with spherical shapes, NH^{4+} ions possess a tetrahedral structure. This unique geometry allows for a more selective intercalation process within the electrode materials, potentially leading to superior power density and extended cycling stability. However, a significant challenge lies in developing electrode materials that can effectively and reversibly accommodate NH^{4+} ions, thereby unlocking the full potential of this technology for high-performance energy storage applications. Herein, we synthesized a multilayered graphene membrane (MGM) with interlayer separation distance suiting the NH^{4+}-ion intercalation. The material characterization of the MGM revealed a stacked structure with a high surface area. The amorphous nature of the graphene membrane delivered oxygen vacancy sites for a flexible hydrogen bond formation between the graphene membrane and NH_4^+-ions. The flexible MGM membrane was electrochemically characterized using 1 M $(NH_4)_2SO_4$ electrolyte and showed electric double-layer capacitance. The membrane could operate at a maximum voltage window of 1 V and deliver a maximum capacitance of 0.66 mF/cm^2 at a scan rate of 20 mV/s. 72 hours of floating test and 1000 cycles of continuous charge-discharge cycles of MGM membrane delivered 100% capacitance retention solving the long-term cycling stability issues of NH_4^+-ion storage.

Keywords: Asymmetric Supercapacitors, Floating test, Manganese oxide, reduced Graphene Oxide, Cycling stability.

Nature-Inspired Nitrogen-Doped Carbon Coating Over a Metal Chalcogenide Nano Seed Embedded Flexible Substrate for a Highly Stable Lithium-ion and Sodium-ion Battery Material

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Enhanced Thermoelectricity in Mg2Si incorporated with Carbon Microfiber and Bismuth

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Thermoelectric power generation, which harnesses distributed waste heat energy, has attracted attention as a sustainable and environmentally acceptable energy source. Mg2Si-based alloys show great potential as thermoelectric materials for converting energy in the intermediate to high temperature range. The thermoelectric performance of Mg2Si has been improved using techniques such as impurity doping, nano-structuring, and alloying. Additionally, they have the potential to lead to a decrease in the weight of thermoelectric generators, which is a crucial characteristic for the automotive industry. This study examines the effects of co-doping with bismuth and trace quantities of the isoelectronic impurity Carbon Microfiber on the thermoelectric characteristics of Mg2Si. This study investigated the effects of varying concentrations of Carbon Microfiber and Bismuth doping on Mg2Si/CFxBiy where x denotes the doping levels of CF (x= 0.01, 0.05) and Y denote the doping level of Bismuth (y=0.03, 0.05). This work produced polycrystalline samples of Mg2Si by Spark Plasma Sintering techniques. Doping Mg2Si with Carbon Microfiber considerably lowered thermal conductivity to 1.724 W/m·K at a temperature of 773 K, marking the lowest thermal conductivity observed to date. Which also considerably affects the electrical conductivity. Consequently, we incorporated Bi as a co-dopant in Carbon Microfiber, which demonstrated a substantial enhancement in electrical conductivity while preserving inferior thermal conductivity relative to singly doped Mg2Si with Carbon Microfiber. The dimensionless figure of merit ZT for the co-doped specimens reached 0.51 at 773 K within the temperature range of 323–773 K.

The Study on Corrosion Effect of Aluminum – Zinc Coated on Steel Surface by the Hot Dipped

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In the construction industry, wall and roof panels commonly used steel coated with aluminum-zinc alloy by hot-dipped. These materials are applied in various environmental conditions, affecting their lifespan due to corrosion until perforation occurs. Surface coating technologies have been developed to enhance performance and are applied in the production process of aluminum-zinc alloy-coated steel, and including the color coating to improved material lifespan and enhance corrosion resistance properties. It consists of three coating layers: a conversion coat layer containing chromium, a primer coat layer containing strontium chromate, and a topcoat of polyester resin. Therefore, this is called pre-painted aluminum-zinc alloy-coated steel.

In this research aluminum-zinc alloy-coated steel with a coating weight of 150 g/m2 was examined, comprising a chromium conversion coating, a strontium chromate primer coating commercially, and a polyester resin topcoat. Classified coating conditions into five types: 1. Without conversion coat, primer and topcoat; 2. Without conversion coat, primer, but with topcoat; 3. Without conversion coat, with primer and topcoat; 4. With conversion coating, without primer, but with topcoat; 5. With conversion coating, primer, and topcoat.

However, when considering corrosion rates of paint coating, the result found that specimens with conversion coat and strontium chromate primer had the lowest average corrosion rate of 0.0134 mmpy, among the tested specimens. This is due to the properties of both chromium-containing coatings. Following this, specimens coated with strontium chromate primer had an average corrosion rate of 0.0192 mmpy, which is faster due to the properties of the chromium trioxide conversion coating that were not applied.

Comparatively, specimens with conversion coating but without strontium chromate primer had an average corrosion rate of 0.0291 mmpy, this is due to the properties of the uncoated strontium chromate. The highest corrosion rate among the tested was 0.0404 mmpy, from specimens with only top coating. This is the fastest corrosion rate, due to the properties of uncoated conversion coat and strontium chromate in the primer, and when compared with specimens that did not have conversion coating, primer, and topcoat, the highest corrosion rate was 0.0805mmpy, due to the absence of surface-coating.

Comparing corrosion rates with production costs (as of August 2022), samples only the topcoat presence 1-time reduction in corrosion rate 45% increased in cost compared to uncoated samples, but it was noted that the surface had oxidation and being unusable. Samples with the conversion coating and topcoat presence 28% reduction in corrosion rate with 1.4% increased in cost compared to those with only the topcoat. Samples with only the strontium chromate primer and topcoat showed 52% reduction in corrosion rate with 4.3% increased in cost. Samples with both the conversion coating and primer, along with the topcoat, presence 67% reduction in corrosion rate with 5.71% increased in cost. However, XRD analysis presence of low-corrosion conditions indicated that the samples with the primer coating contained strontium chromate.

Thus, A combination of conversion coating, primer with strontium chromate, and polyester resin topcoat offers superior corrosion resistance, extending the lifespan of aluminum-zinc alloy coated steel used in construction materials.

Unveiling the design logic of artificial polymer layer on Cu current collector for practical anode free lithium metal batteries

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In response, Anode-free lithium metal batteries have attracted considerable attention due to their high energy density, high safety, low cost, and simplicity of manufacturing. However, this novel system is associated with robust chemical and electrochemical processes, which give rise to thick and heterogeneous solid-electrolyte interfaces (SEI) layer and accelerated degradation of the battery's cyclability. To address these challenges, it is essential to comprehend the reactions at the current collector-electrolyte interface in order to impede the consumption of active lithium and electrolytes through current collector modification. This study presents a strategy to enhance the longevity of anode-free lithium metal batteries. The approach involves the introduction of an ultra-thin polymer layer of 15 nm through a large-area initiated chemical vapor deposition process, which forms a thin SEI layer based on inorganic materials, suppressing electrolyte consumption. The cyclability of the half-cell was increased by more than three times under current densities of 0.5 mA cm^{-2} and 1 mA cm^{-2}. Furthermore, the performance of the anode-free lithium metal battery using NCM811 as the cathode was enhanced by 30 cycles at 50% capacity retention.

Enhancing Selectivity of Peroxidase Mimicking Nanozyme via Ligands Regulation of Ruthenium Single Atom

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Peroxidase(POD)-like nanozymes have gained significant attention due to their potential to serve as substitutes for natural enzymes in various biological applications. Despite this, most nanozymes, including FeNC, perform best in acidic conditions and involve multiple reactions, which limits their broader applicability. These limitations stem from undesirable side reactions, like catalase(CAT)-like and oxidase(OXD)-like reactions. Addressing these challenges, the research focused on the development of ruthenium single-atom nanozymes with ligands (RuNC_Xs), engineered to possess selective peroxidase-like activity.

The findings reveal that RuNC_X with chlorine ligands (RuNC_Cl) not only significantly reduce CAT-like and OXD-like activities but also maintain strong POD-like activity under weak acidic condition. RuNC_Cl were particularly noteworthy, demonstrating a specific activity of 142.32 U·mg^{-1} at pH 6.0—37 times greater than CAT-like activity. This exceptional activity underscores the efficiency of modifying adsorption energy by ligands in catalytic processes. Additionally, RuNC_Cl exhibited remarkable capability in detecting biomarkers, such as glucose, within a paper-based microfluidic sensor system. Importantly, this detection was achieved without laborious procedures like buffer changes, simplifying the operational workflow.

This study significantly contributes to the field by establishing a foundation for the rational design of enzyme-mimicking catalysts. Furthermore, it broadens the potential applications of nanozymes in diverse biological and biomedical fields through improved selectivity and operational conditions.

Achieving durable ammonia oxidation by stabilizing *NH intermediates on Pt-skins at ordered intermetallic Pt-Zn cores

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The transportation of hydrogen derived from ammonia is gaining popularity as the use of hydrogen as a sustainable energy source expands. To produce hydrogen from ammonia without emitting greenhouse gases, catalysts that can electrochemically oxidize ammonia must be developed. Platinum is currently the most active catalyst known, but issues with its dissolution in ammonia-containing electrolytes and the poisoning of the active site by reaction byproducts have prevented platinum from being commercialized. We synthesized intermetallic platinum-zinc catalysts and employed them in the electrocatalytic oxidation of ammonia. The addition of zinc to the catalyst mixture served to stabilize the intermediate *NH, stimulate the dimerization reaction, and mitigate the poisoning of the platinum active site. This approach enabled the production of small-sized particles even after subjecting them to high temperatures during heat treatment. Furthermore, we were able to reduce platinum dissolution, which is more pronounced in electrolytes containing ammonia, and enhance the catalyst's long-term durability by employing an intermetallic compound with a high degree of interatomic coordination as a catalyst for the ammonia oxidation reaction.

Enhancing the Long-term Durability of Multiredox-reaction Electrodes in Sodium-ion Hybrid Capacitors

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The increasing need for high-performance sodium storage materials arises from the limited availability of lithium. As the demand for energy storage solutions grows, lithium resources are becoming progressively constrained, prompting the exploration of alternative materials. Sodium, being more abundant and less expensive than lithium, has emerged as a viable candidate for energy storage applications. However, the development of efficient sodium storage materials is crucial to fully leverage this potential. Materials that employ a multiredox-reaction mechanism present significant promise for application in sodium-ion batteries (SIBs) and sodium-ion hybrid capacitors (SICs). These materials can undergo multiple redox reactions, which can enhance the energy density and cycling stability of the batteries and capacitors. In particular, the ability to utilize multiple redox states allows for more efficient charge and discharge processes, contributing to better performance and longer lifespan of the devices. In this research, we introduce a novel strategy aimed at enhancing the cycling lifespan of multiredox-reaction materials in both SIBs and SICs. The effectiveness of this strategy was rigorously evaluated using a $Na_2VTi(PO_4)_3$@C (NVTP@C) electrode, which incorporates three distinct redox reaction sites (V^{2+}/V^{3+}, Ti^{3+}/Ti^{4+}, and V^{3+}/V^{4+}). This specific electrode composition was chosen due to its potential for high performance and stability. Our electrochemical investigations revealed that excluding the most unfavorable redox reaction of NVTP@C, specifically the V^{2+}/V^{3+} reaction, effectively reduces the voltage hysteresis in Na||NVTP@C half-cells and NVTP@C||AC hybrid ion capacitor systems. Voltage hysteresis, a phenomenon where the voltage during charging differs from the voltage during discharging, can lead to energy losses and reduced efficiency. By mitigating this issue, we were able to significantly extend the cycling lifespan of the devices. Consequently, this strategy, based on a thorough understanding of the behavior and characteristics of multiredox materials, can be utilized to design advanced SIBs and SICs that leverage multiredox-reaction mechanisms. This approach not only enhances the performance and longevity of the devices but also contributes to the broader goal of developing sustainable and efficient energy storage solutions. Through continued research and development, the principles outlined in this study can pave the way for the next generation of sodium-based energy storage technologies, addressing the limitations associated with lithium-based systems and supporting the transition to a more sustainable energy future.

Fabrication of Transparent Conducting Film for Organic Photovoltaic Cells by Carbonization of Polyethylene Thin Film

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In this study, we successfully converted a polyethylene (PE) thin film into a transparent conducting film (TCF). By using thermal oxidative stabilization, we transformed an inherently noncarbonizable PE thin film to withstand the carbonization process, resulting in the formation of a carbon nanosheet (CNS). Remarkably, unlike other CNSs derived from expensive sources, those made from PE, one of the most affordable polymers, featured highly ordered graphitic structures, as verified by Raman spectroscopy and transmission electron microscopy (TEM). These graphitic structures provided the PE-based CNSs with superior electrical conductivity compared to other CNSs and TCFs, without significantly sacrificing other performances. The effectiveness of these CNSs as TCFs was demonstrated through the fabrication of organic photovoltaic cells (OPVs). The OPVs constructed on PE CNSs operated successfully and showed sound efficiencies. Importantly, PE based CNS could be equivalently fabricated based on PE waste. The OPVs constructed on PE waste derived CNS exhibited similar efficiency as the OPVs constructed on pristine PE derived CNS. Therefore, it could be concluded that the carbonization of PE waste could be a potential pathway to add financial value to PE waste. Given that PE waste is the largest polymer waste by volume and is predominantly buried or incinerated, the technology presented in this article offers a promising solution to environmental issues related to PE waste by proposing a viable "upcycling" pathway.

CO_2-Derived Edge-Boron-Doped Hierarchical Porous Carbon Catalysts for Highly Effective Electrochemical H_2O_2 Production

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Electrochemical hydrogen peroxide (H_2O_2) synthesis via the two-electron oxygen reduction reaction (2e- ORR) is considered a promising alternative to the anthraquinone process due to its eco-friendliness and on-site production. Recently, although B-doped carbon (BC) has been suggested as a promising 2e- ORR catalyst, the question of whether BC can further improve catalytic activity by tuning the doping configuration and site still remains unanswered. This work demonstrates CO_2-derived edge-B-doped porous carbon (E-BPC) for highly effective electrochemical H_2O_2 production. Herein, it is revealed that the oxygenated B-doping configurations (BCO_2 and BC_2O) at edge sites are responsible for enhanced 2e- ORR activity and stability. Outstanding mass activity (54.7 A g^{-1} at 0.65 V vs. RHE) is demonstrated with the highest high production rate in a flow reactor among the reported studies, of 24.3 mol $gcat^{-1}$ h^{-1}. The faradaic efficiency of the E-BPC was maintained (~82%) for over 100 h without performance degradation.

A study on formability of rear floor applied with lightweight vibration damping steel plate material

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In response to the escalating global demand for environmental sustainability, the automotive industry is increasingly prioritizing compliance with fuel efficiency regulations and the transition to eco-friendly vehicles as pivotal strategies to reduce greenhouse gas emissions associated with global warming. This paradigm shift has catalyzed a substantial increase in the utilization of lightweight materials within automotive manufacturing, aimed at enhancing fuel efficiency and minimizing the environmental footprint of vehicles. In automotive body construction, weight reduction is predominantly achieved through the extensive use of aluminum materials. However, the integration of ultra-high-strength steel sheets remains indispensable for components that necessitate the primary structural integrity of the vehicle to meet stringent safety regulations. In this context, vibration damping steel plates are garnering significant attention for their multifaceted benefits, including carbon dioxide emission reduction, weight minimization, and enhancements in NVH (Noise, Vibration, and Harshness) performance. Vibration damping steel plates are characterized by a sandwich structure, where viscoelastic polymer adhesives with superior damping properties are utilized to attenuate vibrations in thin sheets. The automotive industry is actively exploring the application of these materials across various components. This study focuses on the formability assessment conducted via sheet metal forming analysis on rear floor components, which have been lightened in comparison to mass-produced counterparts through the use of high-strength damping steel plates. The lightweight rear floor is fabricated using damping steel composed of 5052 aluminum alloy bonded with a viscoelastic polymer adhesive, undergoes cold press forming. To scrutinize the forming process of the rear floor, forming simulations and formability evaluations were conducted utilizing the commercial software AutoForm. The mechanical properties of the damping steel sheet were meticulously identified and incorporated through tensile tests to ensure precise material characterization. The forming analysis examined sheet metal deformation behaviors, including fracture, wrinkling, and excessive thinning, culminating in the determination of the optimal die face design. Subsequently, the mechanical integrity of the lightweight rear floor, incorporating damping steel, was rigorously assessed, and the forming process was validated through comprehensive optimization. This research was supported by "Regional Innovation Strategy (RIS)" through the National Research Foundation of Korea(NRF) funded by the Ministry Education(MOE)(2022RIS-006)

DAY 3 September 25, 2024

ROOM A

Session: Biomaterials, Bioengineering and Bio-related Applications

Innovative Approaches for Processing Drug-Containing Coatings and Drug Delivery Devices

Roger Narayan, North Carolina State University, USA

Semiconducting Polymer Nanoparticles: Soft Materials to Overcome Hard Challenges in Neuroengineering

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Abstract

Implantable neurostimulation devices play a key role in treating many serious injuries and diseases by providing a direct therapeutic link to the nervous system. The main obstacles to further translation of these devices include a low biocompatibility, a mechanical rigidity that is poorly matched with soft tissue, a requirement for external power and indiscriminate tissue activation. Here we report a new materials nanoengineering approach to simultaneously address all these issues and enable highly precise wireless optical neurostimulation using semiconducting polymers.

Organic semiconductors were transformed into biocompatible aqueous nanoparticle suspensions using colloidal chemistry. Neuroprotective chemicals were embedded into these electroactive nanoparticles by immersion in the aqueous inks. We fabricated these inks into pixelated arrays using inkjet printing and demonstrated their biocompatibility using immunolabelling with a neuronal marker. Electrical responses of neurons to stimulation with the arrays were measured using patch clamp electrophysiology. The nanoparticle inks successfully formed multifunctional arrays that released neuroprotective factors on demand. Neurons cultured onto these multifunctional arrays showed substantially improved connections to the material interface, which exhibited exceptional anatomical and functional biocompatibility. Electrophysiology recordings demonstrated a paradigm-shifting result; the membrane potential of neuronal cells was able to be controlled via capacitive coupling using purely optical neurostimulation of the multifunctional arrays without any external wires or power. Our results reveal that nanoengineering organic conductors can overcome the gap between the electronic and biological worlds, enabling a new pathway for highly precise wireless neural stimulation.

Fabrication and Characterization of Biaxially Expanded Polymeric Tubes for Coronary Stent Application

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Formulation and characterization of a novel Quercetin conjugated MgO nanoparticle for cancellous alveolar bone tissue regeneration

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Teeth loss is mostly linked with the loss of alveolar bone, which is the supportive structure of teeth. The complex structure of cancellous alveolar bone causes a great challenge for the researchers to develop an effective alveolar bone regeneration therapy. The use of nanoparticles in dental implants to reduce implant infection, free radical formation and time of healing is a promising option for speedy recovery of defect alveolar bone tissue. The formulation of a potential nanoparticle is, therefore, highly demanding for dental implants. Quercetin, a flavonoid, is popularly known for its strong antimicrobial, anti-oxidant and osteogenic properties. As reported, modification of quercetin (Qr) functional groups in blood plasma hinders the bioavailability of this phytocompound at the defect site. Therefore, there is a need for conjugation of Qr with a molecule which can avoid functional modification in Qr. In this context, the metallic magnesium oxide (MgO) nanoparticle which is well-known for its osteogenic activity can be conjugated with quercetin to improve its bioavailability. In the present research, green synthesis of quercetin conjugated MgO, referred as Qr-MgO as a novel nanoparticle was successfully developed, wherein Qr was used as a reducing agent for MgO. FESEM micrographs revealed speherical structures of of MgO and Qr-MgO nanoparticles with particle size of 44.42±0.008 nm and 90.01±0.001 nm respectively. Elemental analysis validated the presence of Mg in Qr-MgO nanoparticle. FTIR analysis confirmed the Mg-O bond vibration with a slight shifting in the peaks and specific Qr peaks in Qr-MgO nanosphere. From X-ray diffractogram the crystalline structure of nanoparticle with presence of distinguished MgO and Qr peaks were observed. The UV-VIS spectrum scanning of nanoparticle showed peaks at 264 and 388 wavelengths which are between the spectrum of MgO nanoparticle and quercetin molecule, confirming the conjugation of MgO particle with Qr. The anti-oxidant property of the MgO nanoparticle was tremendously enhanced measuring 84.52±1.33% when conjugated with Qr. The antimicrobial activity of the Qr-MgO nanoparticle was significantly higher compared to MgO nanoparticle against *Escherichia coli* (gram-negative) and *Staphylococcus aureus* (gram-positive) bacteria. Herein, the impact of MgO and Qr-MgO nanoparticles on Human Osteoblast like Saos-2 cell was examined via MTT assay and cell viability rate. The Saos-2 cells exhibited remarkably higher viability and proliferation rate when cultured in Qr-MgO nanoparticle treated samples than the MgO treated sample. Overall, it was demonstrated that Qr-MgO nanoparticle can be acted as an ideal nanoparticle for reconstruction of cancellous alveolar bone tissue.

Keywords:, Anti-microbial, Anti-oxidant, Cancellous alveolar bone, Magnesium oxide, Nanoparticle, Quercetin

Advanced 3D Bioprinting of Iron (III) Crosslinked Carboxymethyl Cellulose Bioinks for Enhanced Soft Tissue Regeneration

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The emergence of three-dimensional (3D) bioprinting technology has enabled the precise assembly of complex constructs for soft tissue engineering applications. Among various biopolymers, carboxymethyl cellulose (CMC) has garnered attention as a promising biomaterial for synthesizing bioinks. Nevertheless, the limited ability to maintain post–printed stability of CMC necessitates its physical blending and/or chemical crosslinking with other polymers. In this study, CMC was combined with xanthan gum (XG) and hyaluronic acid (HA) to develop a hybrid bioink, integrating the printability of CMC and XG with the cell support properties of HA. Ionic crosslinking with ferric ions was employed post-printing, utilizing the coordination between iron (III) cations and the carboxylate groups of the polymers to enhance mechanical strength and long-term stability. The bioprinting of these ionically crosslinked bioinks demonstrated excellent viability (over 95%) and preserved morphology of encapsulated immortalized human epidermal keratinocytes and human foreskin fibroblasts. Overall, this research underscores the potential of ferric – crosslinked CMC/XG/HA hydrogels as novel and advanced bioinks for soft tissue regeneration.

Water-based Synthesis of Metal-Organic Frameworks (MOFs) for Carbon Neutral Society

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Development of Metal-Organic Frameworks as a Biosensor Matrix for Detecting Infectious Diseases Caused by Viruses

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Metal-organic frameworks, or MOFs, are a type of porous material that have advantages such as a high surface area, abundant porosity, and surfaces that can be easily modified. MOFs with transition metals become interesting to utilize in electrochemical biosensors, especially if the MOF surface is terminated with metals as active sites, resulting in a high surface area with abundant available active sites. Several studies have successfully utilized MOFs as biosensor materials, particularly for virus detection. HKUST-1-based MOFs with a one-dimensional structure have been successfully used to detect the dengue virus. Modification was performed using high concentrations of triethanolamine to obtain a 1D structure with abundant metal centers. This strategy resulted in a biosensor with a detection limit of 0.9 pg/mL. Surface modification can also be performed by adding other transition metals to provide a variety of active sites. Nickel and copper were used as modifiers for HKUST-1. The presence of these metals reduced the detection limit to 0.7 pg/mL and 0.5 pg/mL, respectively. Another virus successfully detected using MOFs is Hepatitis B. Other copper-based MOFs were also modified to detect the Hepatitis B virus. MOFs with a spherical structure had high sensitivity and a detection limit of 730 pg/mL. Additionally, HKUST-1 was also used to detect Hepatitis B with a detection limit reaching 0.89 pg/mL. Moreover, MOFs can also be utilized in virus detection using optical techniques such as surface plasmon resonance (SPR). For example, our group successfully developed a MOF with zirconium metal, which was used as a material to modify a gold chip for detecting the COVID-19 virus. With this technique, the detection limit for the COVID-19 virus is 10.085 × 105 viruses/mL. These research results demonstrate the high potential of MOFs for use in healthcare, particularly in biosensors.

Keywords: *Biosensors, electrochemical, metal organic frameworks, virus, surface plasmon resonance.*

Molecular and Nanoarchitecturing Strategies of Functional Porous Materials for Catalytic Applications

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Functional porous materials, both organic and inorganic, offer a wide array of nanoarchitectures and possess highly promising properties. These materials can be synthesized through various methods, including molecular design and control, surface coating, etching, and complexation. Each of these synthesis techniques allows for precise control over the material's structure and functionality. These functional porous materials exhibit excellent physical and chemical properties, making them versatile and effective platforms for a multitude of energy and environmental applications. For instance, they have shown great potential as electrocatalysts, facilitating reactions with high efficiency and stability. In the realm of CO_2 conversion, these materials are invaluable, offering effective solutions for carbon capture and utilization, thereby addressing pressing environmental concerns. Furthermore, they are also effective in the detoxification of chemical warfare agents, providing a critical means for decontamination and protection.

The versatility of these materials is further enhanced by their tunable nanostructures. By adjusting their nanoarchitecture, these materials can be optimized for specific applications. This involves enhancing the number of reactive sites, improving diffusivity, and tailoring the material's reactivity and affinity for particular reactants. Such modifications enable the functional porous materials to be tailored precisely for the desired catalytic reactions or mechanisms, thereby expanding their applicability and effectiveness across various fields.

In this study, we present several strategies for synthesizing functional porous materials through molecular and nanostructural control of metal-organic framework (MOF)-based materials and their composites. By implementing effective approaches and optimizing molecular and nanostructures, we aim to enhance the properties of these materials for applications in energy and catalysis, including electrochemical reactions, CO_2 cycloaddition reactions, and the detoxification of chemical warfare agents (CWAs). Precise control of the molecular structure can significantly enhance the reactivity of specific catalysts by increasing their affinity for reactants or by incorporating multifunctional groups. Moreover, appropriate nanoarchitecturing can increase the number of active sites and significantly improve diffusivity, thus enabling a wide range of catalytic applications.

In summary, the development and optimization of functional porous materials through advanced synthesis methods offer significant potential for energy and environmental applications. Their inherent properties and adaptable nanostructures make them a robust platform for addressing contemporary challenges in catalysis, CO_2 conversion, and detoxification.

Nanoarchitecturing of metal-organic frameworks

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Nanoarchitecturing of metal-organic frameworks (MOFs) has attracted great interest due to its ability to expose surface and active sites, shorten diffusion pathways, and improve electrical conductivity. However, surfactants or modulators are usually employed to synthesize micro-/nanosized MOFs with well-defined shapes often leads to new pollution of products, resulting in performance degradation. To address this issue, we propose a recrystallization strategy to obtain a nanoarchitecture Zn-based MOF by exploiting the weakly coordinating nature of alcohols in ZnBTC. The recrystallized ZnBTC successfully results in a unique nanoarchitecture with abundant nanowires of various aspect ratios. DFT calculations on the chemical potential and hardness of alcohols explain the impact of different alcohols on the recrystallization of ZnBTC. The as-prepared nanowire ZnBTC is converted to its carbonaceous form, demonstrating a unique nanoarchitecture consisting of numerous nanowires to achieve promising energy storage performance as a supercapacitor electrode.

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Crystal structure and chemical bonding studies using convergent-beam electron diffraction

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Recent advancements in the development of nanoscale functional materials have increased interest in studying the origins of their enhanced physical properties at the most fundamental levels. This means understanding their crystal structures and chemical bonding states. Among the various diffraction techniques available, convergent-beam electron diffraction (CBED) is advantageous for such studies because it uses a nanometer-sized electron probe, enabling the acquisition of diffraction intensity from nano-localised, defect-free crystalline regions [1, 2].

In this presentation, I will introduce the CBED technique and highlight its advantages. The first part of the talk will focus on the crystal structure analysis of $(Sr_{1-x}Ba_x)_2Nb_2O_7$ [3] using CBED. In the latter part, I will explore the quantitative aspects of CBED, sharing a novel strategy that we developed to improve precision and sensitivity in chemical bonding studies [4]. Additionally, I will discuss recent research conducted by our group in this area.

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The Computational PHFGMC Micromechanical Nonlinear Analysis for Aerospace Composites, Biomaterials, and Engineered Tissues

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The parametric high fidelity generalized method of cells (PHFGMC) micromechanical framework is presented for the three-dimensional (3D) modeling of multi-phase heterogeneous materials. This framework enables nonlinear and strain-softening constitutive formulations, allowing for thermo-mechanical multi-scale simulations of aerospace composites and soft-to-hard tissues. Within the PHFGMC framework, the multi-phase heterogeneous composite is assumed to possess a periodic microstructure, with detailed interactions between the constituents explicitly recognized. For multi-phase soft tissues, the constituents are considered hyperelastic, and the overall behavior of the composite tissue is established along with the field distributions within the constituents. The PHFGMC framework is implemented within a commercial finite element (FE) code to perform multi-scale analysis of composite materials and structures.

A wide range of PHFGMC computational material modeling applications will be presented and discussed, including the analysis of soft arterial tissues, vertebral trabecular bones, and collagen-alginate biomaterials. Additionally, the analysis and design of ceramic matrix composites (CMC) and fiber-reinforced polymeric (FRP) composites will be demonstrated.

Furthermore, a new coupled micromechanical damage formulation is introduced by directly integrating the phase-field (PF) theory for fracture with the PHFGMC micromechanical model. This combined PHFGMC-PF approach is proposed for progressive damage analysis of multi-phase heterogeneous media subjected to general multi-axial stress. New variational equations couple the macro/micro deformation and PF damage fields within the discrete finite volumes (subcells). An iterative computational solution is also introduced for the overall nonlinear equations. Two PF damage laws are implemented, and the proposed PHFGMC-PF model is verified and compared to published finite-element-PF (FEPF) results for single-edge crack problems under tension and shear. New PHFGMC-PF progressive damage simulations are presented for carbon fiber-reinforced composites, showing good agreement with experimental data.

The PHFGMC framework's versatility is further illustrated through its application to soft and hard tissues. Nonlinear and strain-softening constitutive modeling and large deformation formulations are effective in simulating damage in aerospace composites and the mechanical behavior of tissues. For multi-phase soft tissue, hyperelastic constituents and the overall composite behavior are modeled, while for hard bone tissue, the HFGMC-based multi-scale micromechanical model predicts the effective and damage mechanical behavior of vertebral trabecular bones (VTBs). Hierarchical VTB micromodeling involves three levels: nano-scale 3D-HFGMC for mineral collagen fibrils, sub-micron scale 3D sublimate-model for multi-layered lamellae, and micron-scale 3D-HFGMC for porous VTB microstructures. The soft tissue HFGMC model is calibrated with experimental data and compared to the anisotropic constitutive model by Holzapfel and coworkers. Similarly, the hard-tissue HFGMC model uses micro-computed tomography (µCT) scans to predict overall anisotropic properties for native VTBs, compared with reported values in the literature.

In conclusion, the PHFGMC is demonstrated as a novel effective, viable micromechanical modeling approach for various applications, including soft and hard tissues and various composite materials, establishing its utility in advanced material analysis and design.

Predicting the dynamic properties of materials

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Accelerating the Discovery and Design of Novel Materials by ALKEMIE

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The development of high-throughput automation integrated-computations and data mining algorithms based on material databases and artificial intelligence algorithms is crucial for accelerating the discovery and design of novel materials. In this talk, I will present an open-source distributed computational platform named Artificial Learning and Knowledge Enhanced Materials Informatics Engineering (ALKEMIE) which is based on the AMDIV (automation-modular-database-intelligence-visualization) design concepts. Meanwhile, I will present ALKEMIE-MatterDB, which contains multi-type materials database of structure, task, workflow and material property. Combining with the power of supercomputing, ALKEMIE enables the rapid deployment of artificial intelligence algorithms in the design of new materials. Finally, a few examples of the discovery and design of novel materials using ALKEMIE will be demonstrated.

Biography:

Zhimei Sun is a Cheung Kong Scholar Chair Professor at School of Materials Science and Engineering of Beihang University, China. She received her Ph.D. of Materials Science from Institute of Metal Research (CAS) in 2002, and after which she worked at RWTH Aachen University (Germany) and Uppsala University (Sweden) from 2002 to 2007, and at Xiamen University (China) from 2007 to 2013. Her research includes phase-change memory materials, high-performance structural materials and 2D transition metal carbides/borides. She has published 300 SCI papers and has been ranked in the Most Cited Chinese Researchers by Scopus in the past four years.

Mesoscale Modeling for Predicting Mechanical Properties of Hemp Fiber Composites Considering Yarn Variability

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The utilization of natural fibers in composite material production has gained significant attention across diverse industrial sectors, including automotive, aerospace and construction, owing to their advantageous characteristics of low density, sustainability, and environmental compatibility. Hemp fibers, in particular, demonstrate considerable potential as a substitute for synthetic fibers, such as glass, in structural applications due to their comparable specific strength. However, the widespread implementation of hemp fibers remains constrained by the inherent variability in their mechanical properties, which subsequently impacts the overall composite material performance. This variability is primarily attributed to the intricate morphology of the yarn structure. This study employs a Representative Volume Element (RVE) mesoscale model of plain-woven hemp fabric, constructed using geometric data derived from micro-computed tomography (micro-CT) scans, to quantify the variability in mechanical properties of hemp fiber-reinforced laminates. While micro-CT scan-based virtual models can be applied in finite element analysis and offer high fidelity in mechanical property prediction, they are associated with substantial computational complexity, cost, and time constraints. To address these limitations, a simplified mesoscale yarn model represented by one-dimensional beam elements embedded within a three-dimensional matrix model is proposed, thereby circumventing the intricacies of fully-detailed models. Results from finite element analysis revealed that the simplified model can accurately predict mechanical properties, including elastic modulus and fiber-direction strength, closely matching results from the virtual model while significantly reducing computational time and modeling complexity. Further investigation into the effects of hemp yarn morphology on the mesoscale model demonstrates that variations in yarn width and spacing significantly impact mechanical properties due to alterations in fiber volume fraction within the laminate. Increased fiber volume fractions enhance material properties by up to 16%. Conversely, changes in yarn height and simultaneous variations in yarn width and spacing do not affect fiber volume fraction but influence the crimp angle of the fiber. Higher crimp angles in the hemp yarn fabric result in a 12% reduction in material properties. Furthermore, the simplified fiber modeling approach with 1D beam elements facilitates the study of yarn misalignment effects across multiple plies in the laminate, which can occur due to forming processes, on mechanical properties. This simplified circular fiber modeling approach can be extended and further developed to investigate damage behavior and apply to other natural fiber-reinforced composite materials.

Liquid Metal Derived Functional Nanointerfaces

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Adsorption Energetics and Thermodynamics on Semiconductor Surfaces Based on Machine Learning

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Accurately understanding the atomic-level structure of semiconductor surfaces under growth conditions is fundamental to comprehending growth mechanisms. Once the surface structure is determined, adsorption and desorption energies, as well as surface migration potentials, can be accurately calculated. This enables mesoscale growth simulations based on Monte Carlo molecular simulation methods [1]. In the field of semiconductor surface research, surface phase diagrams, which relate growth conditions, such as temperature and pressure, to thermodynamically stable surface structures, have been constructed based on first-principles calculations and statistical mechanics [2]. However, application to large-scale surface structures has been impossible because the number of candidate structures for first-principles calculations becomes enormous. In this study, we overcome this challenge by utilizing Bayesian optimization. Additionally, we develop a methodology to explore mixed states of multiple types of surface reconstructions. This signifies a shift from traditional theoretical surface phase diagrams, which only considered the entropy of the gas phase and lattice vibrations, to an accurate consideration of surface configurational entropy. When applying the proposed method to the GaN surface, a stabilization rule known as local electron counting was observed [3]. Furthermore, as a generalized concept of this rule, we propose an analysis method for surface adsorption configurations based on the Ising model [4]. This allows us to obtain the thermodynamic partition function of the surface system and calculate thermodynamic properties. The series of approaches we propose is not limited to the application to the GaN surface; it can be adapted to analyze the precise properties of various semiconductor surfaces, such as surface energy, adsorption energy, and migration energy, depending on experimental conditions.

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Intramolecular triplet-triplet fusion in Benzimidazole-decorated Bisanthracene and Its Application for Blue Organic Light-emitting Diode

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Organic light-emitting diode (OLED) is a main-stream display technology, which has been widely used for the applications of smart watch, cell phone, tablet, laptop, and television. Among three primary colors, blue OLED exhibits lowest device efficiency and shortest operation lifetime compared to red and green one, because of its wide bandgap nature [1]. Although red and green phosphors have achieved great success in efficiency and lifetime for OLED mass production, blue phosphorescent device cannot meet the lifetime criteria. Upon electrical excitation, 25% singlet and 75% triplets are generated in an OLED. In a triplet-triplet fusion (TTF) material, two triplets may fuse to one singlet for light emission. Although the theoretical limit of internal quantum efficiency (IQE) for blue TTF-OLED is lower than that of phosphorescent and thermally activated delayed fluorescence (TADF) devices, its operation lifetime is much longer which is acceptable for display applications of consumer electronics. Hence, in commercial blue OLED, anthracene derivatives with TTF characteristics are typically used in the emitting layer (EML).

However, in TTF materials, it is not straightforward for two triplets from two molecules fusing to one singlet. Suitable molecular packing is crucial. Obviously two anthracene units from two molecules must be close enough for TTF process. However, if they are too close, excimer may be formed which generates another competing relaxation channel. Not only distance between anthracene units, different packing geometries also affect the TTF efficiency significantly. For achieving a fixed packing configuration between two anthracene units, we proposed to use bisanthracene backbone, which consisted of two anthracenes separated by a phenylene ring, for achieving intramolecular TTF effect [2]. Besides, this molecule was decorated by benzimidazole end-group for improving the photoluminescence quantum yield (PLQY), as high as ~90% both in solution and thin film. When using this material, named as DiAnBz, as the emitter of blue OLED, 8.3% in external quantum efficiency (EQE) was achieved. When DiAnBz concentration was down to 1% in the EML of the blue OLED, delayed emission was still observable which proved the existence of intramolecular TTF process. In this device, spectral peak of electroluminescence was at 442 nm, and the CIE coordinates were at (0.148, 0.070) for deep-blue emission from anthracene moiety. Besides, high horizontal dipole ratio of this emitter was as high as 90% due to the planar structure, which also boosted up the EQE.

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Metasurfaces for Microwave Beam Steering

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Preparation and Application of Liquid Metal-Based Heterocomposites

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A Novel Quantum Computing Platform: Superconducting Bosonic Quantum System

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Layered Semiconductors for Electronic Sensing and Optoelectronic Applications

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Flexible Silicon Carbide (SiC) electrodes for implantable devices

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Flexible and stretchable devices for long-term implantable applications represent an emerging area of research. These devices offer excellent mechanical flexibility to achieve better conformal contact with internal organs and tissues, accommodating the large deformations of internal organs such as lungs, bladders, and stomachs. However, conventional materials like platinum and gold, commonly used in these devices, react with biofluids in the human body, producing harmful chemicals for tissues and shortening the lifespan of devices. Therefore, developing long-lasting electrodes that can remain inside the body for several years is a significant challenge for chronic implantable devices. Among several material systems, Silicon Carbide (SiC) emerges as a promising candidate due to its superior physical and chemical properties that have been widely utilized for extreme environmental applications, including high temperatures and corrosion. Built on our established technologies on the growth of SiC nanothin films on a Si substrate, this study focuses on manufacturing techniques for SiC-based flexible and stretchable electrodes for long-term implantable purposes. By applying the mechanical stamping method, we transfer SiC electrodes and form metal interconnects on a polyimide substrate. The entire structure is then encapsulated in another thin polyimide layer. Using the mechanical buckling approach, we selectively bond the SiC/polyimide films with a pre-strained Ecoflex substrate, creating 3D SiC structures upon strain release. The bucked configuration offers excellent mechanical stretchability of up to 100% strain, effectively overcoming the limitation of intrinsic SiC materials. Temperature and impedance sensing demonstrated the potential of these devices in monitoring biophysiological signals, showcasing their promise for long-term implantable applications.

Nanotechnology-Driven Personalised Medicine: Nano-Sensing Systems for Early Disease Detection and Trace Biomarker Profiling

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Vertical Graphenes: Synthesis, Functionalization and Applications

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Vertical graphenes (VGs) represent an aggregate of standing few-layer graphenes. This kind of carbon nanostructure is also called as carbon nanowalls (CNWs), carbon nanoflakes, and graphene nanowalls. VGs and similar carbon nanostructures are basically self-assembled network of few-layer graphene “walls” standing almost vertically on the substrate to form 3D maze-like structure as a porous membrane with distorted honeycomb pattern. VGs are characterized by self-supported few-layer graphene sheets with open boundaries, standing almost vertically on the substrate. They possess large specific surface area and ample spaces surrounded by vertical graphene walls. Therefore, VGs can be used as electrode for capacitors. VGs can also be used as electrode for electrochemistry, since reported potential window for VG electrode is nearly 3 V, which is as wide as that for boron-doped diamond electrode. The structure of VGs with large surface area can be suitable for the platform in electrochemical and biosensing applications.

VGs and related materials can be synthesized by PECVD on heated substrates (600-800 ˚C) using methane and hydrogen mixtures on a variety of substrates including Si, SiO_2 and metals. In the typical case of VG growth, after the nucleation, the height of VGs increases almost linearly with the growth period, while the thickness of each sheet and interspaces between adjacent sheets are almost constant. From TEM observation, each sheet is composed of nanographene domains. These domain boundaries and graphene edges are chemically reactive, and metal nanoparticles such as Pt nanoparticles stick selectively at the grain boundaries and graphene edges. Therefore, combined with surface functionalization, VGs can be suitable as platform in electrochemical and bio applications. Towards the emerging applications, the surface of VGs is functionalized, in other words, modified with several types of surface termination and decoration with metals/metal oxides and biomolecules to add new features to VGs as composite catalysts. We have carried out whole surface decorations of VGs by several methods including Pt nanoparticle formation by the reduction of Pt salt precursors; Pt and TiO_2 nanoparticle formation by metal organic chemical fluid deposition using supercritical CO_2 with organometallic precursors; ZnO, SnO_2 and NiOx nanoparticle formation by thermal decomposition of aqueous solutions containing metal acetates and nitrates. In addition, glucose oxidase was selected as the enzyme, and was immobilized on the surface of VG to be used as electrode materials for glucose fuel cell. Electrochemical experiments demonstrate that VGs can be promising electrode materials for electrochemical sensing, biosensing and energy conversion applications.

Design and Performance Study of Sb-based Anode Materials for Sodium-ion Batteries

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Over the past decades, sodium-ion batteries (SIBs) have been developed vigorously and are regarded as the most promising supplementary energy storage technology to lithium-ion batteries. Exploring an effective anode electrode with high capacity and high-rate performance is the key for developing future commercial SIBs. Recently, transition-metal sulfides, and sodium metal have been applied as potential anode materials.

First, Sb-doped copper sulfide hollow nanocubes coated with carbon shells (Sb-CuS@C) was designed and constructed as anode nanomaterials in sodium-ion batteries. Thanks to the intrinsic good electron conductivity and chemical stability of carbon shells, Sb-CuS@C possesses a higher overall electron transfer as anode material, avoids agglomeration and structural destruction during the cycling. As a result, the synthesized Sb-CuS@C achieved an excellent reversible capacity of 595 mAh g^{-1} after 100 cycles at 0.5 A g^{-1} and a good rate capability of 340 mAh g^{-1} at a higher 10 A g^{-1}. DFT calculations clarify that the uniformly doped Sb would act as active sodiophilic nucleation sites to help adsorbing sodium-ion during discharging and leading uniform sodium deposition. This work provides a new insight into the structural and componential modification for common transition-metal sulfides towards application as anode materials in SIBs.

Second, we designed a 3D Cu foam current with dual-modification of antimony and fluorine doping (Sb-doped CuF_2@Cu) can in situ form an inorganic-rich SEI layer through the process of sodium deposition. The SEI layer is composed of an outer layer near the electrolyte that contains Sb^{3+} ($Na_2Sb_4O_7$) and an inner layer that is rich in NaF. The outer layer is beneficial for Na^+ conduction, homogenizing Na^+ flux, and serving as a buffer layer, while the NaF inner layer prevents continuous reduction reactions and homogenizes the electric field, further suppressing dendrite growth. This work introduces fluorine and antimony through a simple one-step displacement method, which is then converted into an inorganic-rich SEI layer, as evidenced by detailed X-ray depth profiles and Ex-TEM. Theoretical calculations and in situ optical microscopy have shown that the inorganic-rich SEI enables rapid Na^+ transfer across the entire 3D framework to enable densely filled. Owing to these benefits, the Sb-CuF_2@Cu@Na anode combined with the $Na_3V_2(PO_4)_3$ cathode produces a full battery with a long service life of 1000 cycles at 5 C. This work presents a novel solution to the dendritic growth problem of Na metal anode.

Furthermore, we facilitated the formation of an inorganic/organic SEI and sodium affinity site (Zn_3Sb_4), which not only provides a stable barrier against electrolyte decomposition but also promotes uniform Na^+ transport, thereby enhancing the overall cycling stability of the anode. By optimizing the interfacial composition and structure, the resulting Sb-ZnF_2@Na anodes exhibit dendrite-free sodium deposition, significantly enhanced electrochemical performance, and improved long-term stability. The symmetrical Na||Na cells boasting an inorganic/organic SEI and sodium affinity site have an extended cycle life of 2000 hours at 6 mA cm^{-2}, 3 mAh cm^{-2}. The findings provide valuable insights into the design of advanced sodium metal anodes for next-generation SIBs.

Carbon Recycling by Microwave Ceramics Synthesis

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Revising Magnetic Features in a New 2D vdW Ferromagnet: Fe_3GaTe_2

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Fe_3GaTe_2 is a 2D vdW layered material with an intrinsic ferromagnetism identified by above-room temperature Curie temperature (*Tc*) and a robust large perpendicular magnetic anisotropy (PMA). Previous studies have shown that 2D vdW ferromagnets are promising candidates for many magnetoelectronic devices and next-generation spintronic applications. However, these 2D materials must be stable at room temperature with long range magnetic order for the majority of spintronics applications [1-3]. Theoretically, long-range ferromagnetism hardly exists in 2D materials because of thermal fluctuation and reduced spatial dimensionality but long-range order can be stabilised by the anisotropy-driven spin-wave excitation gap. Despite this, no intrinsic 2D vdW ferromagnetic crystals such as CrI_3, $Cr_2Ge_2Te_6$ and Fe_3GeTe_2 have ordered magnetic states at room temperature. To date, the 2D vdW ferromagnet with the highest Curie temperature is Fe_3GaTe_2, which has *Tc* (~350-380K), a high saturation magnetic moment (40.11 emu/g) and large PMA energy density (~4.79 X $10^5 J/m^3$) with hexagonal structure of space group $P6_3/mmc$ ($a = b = 3.9860$ Å, $c = 16.2290$ Å, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$) [2].

The study aims to revise magnetic properties of Fe_3GaTe_2 by investigating its magnetic structure. Initial measurements of polycrystalline samples, obtained by manual grinding of bulk crystals, using neutron powder diffraction (wavelength 2.41Å, Echidna diffractometer at ACNS), revealed a sharp peak near $q=0.25Å^{-1}$ at 4K, which transitioned into a broad peak at 400K. However, Small Angle Neutron Scattering with Bilby indicated that this peak was an artifact of measurement limitations rather than a genuine magnetic signal. Further investigations using the Thermal Triple Axis Spectrometer with Taipan (wavelength of 2.345 Å) revealed at least one new magnetic peak arising below 100K. To identify different magnetic phases more precisely, single Fe_3GaTe_2 crystal will be analysed using neutron single crystal Laue diffractometer with Koala later this year.

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Silica Confinement for Stable Co−Cu Alloy Nanoparticles in Nitrogen-Doped Carbon for Enhanced Hydrogen Evolution

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Investigation of the Solid Electrolyte Interphase and Interfaces in FSI-based Ionic Liquids with Various Cations for Na-ion Batteries

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Advanced Na-ion batteries are a promising technology as an alternative/complementary option to Li-ion batteries. However, undesirable solid electrolyte interphase (SEI) and dendrite formation are among the least understood components of rechargeable batteries including Na-based batteries and main challenges for enabling their full potential [1]. Ionic liquids are a class of promising electrolytes with stable electrochemistry and scope for tailoring their properties for high performance Na-based batteries. Interfacial structuring, SEI characteristics, and the correlation between bulk properties and near-electrode properties of these electrolytes are not yet fully understood.

Herein, novel approaches including In-situ Raman spectroscopy, electrochemical quartz crystal microbalance experiments (EQCM) and differential capacitance measurements have been employed to elucidate the interface and SEI formation in Na-based batteries working with liquids. The results have been correlated with cyclic voltammetry measurements to correlate the interface properties with electrochemical behaviour of mentioned electrolytes. C3mpyrFSI:(10)mol%NaFSI and P111i4FSI:(10)mol%NaFSI electrolytes were prepared from the class of pyrollidinium, phosphonium based ionic liquids, respectively. Raman spectroscopy was conducted on electrolytes near the Cu electrode surface at different potentials using a 633nm laser. EQCM measurements have been conducted on gold electrode surface to probe the mass deposition on the electrode surface under constant current electrochemical measurements employing the selected electrolytes. Differential capacitance measurements have been conducted to investigate the effect of using various cation on electrical double layer behaviour [2]. Comparing the Raman spectra of the C3mpyrFSI:42mol%NaFSI and P111i4FSI:42mol%NaFSI electrolytes shows different peak areas and positioning for the FSI anion at open circuit potential (OCP). Moreover, in-situ Raman results for C3mpyrFSI:10mol%NaFSI and P111i4FSI:10mol%NaFSI show different interfacial ion coordination environments and different SEI peaks upon applying various potentials. According to EQCM results, the mass deposited during SEI formation differs between the two systems, with less mass deposited using the P111i4FSI:(10)mol%NaFSI system, which may suggest different SEI thicknesses. Additionally, the mass change at OCP after turning off the potentiostat suggests a soluble SEI model.

Overall, this study can provide new understanding of the role of interfacial structuring in ionic liquid-based electrolytes on SEI formation. This research is ongoing, and the future direction seeks to use these advanced techniques to investigate electrode interfaces and SEI formation in other ionic liquid-based electrolytes.

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Functional Nanocoatings in the Modern Age

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Waterborne polymer nanocomposites: design and application

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Polymer nanocomposites continue to attract significant research and industrial commercial interest alike.[1] Polymer nanocomposites bring "the best of both worlds" (polymer and filler) making them highly attractive for a range of applications including sensing, energy storage, biomedical engineering, insulation, shielding, environmental remediation and catalysis. Polymer nanocomposites exhibit distinct physicochemical properties that are otherwise inaccessible using individual components alone. It is well-established that the efficiency of polymer nanocomposites regardless of the application primarily depends on the distribution of fillers within the polymer matrix. The problem of heterogeneous distribution is particularly challenging when using nano-dimensional fillers (nanoparticles and nanosheets). Furthermore, control over the distribution of fillers becomes more challenging when polymer nanocomposites are moulded into two-dimensional (2D) films and coatings. In this talk, different synthesis and fabrication strategies aimed at controlling the arrangement and distribution of fillers in 2D films leading to some unprecedented final properties will be discussed.[2-6] It will also be demonstrated that simple adjustments in synthesis strategy and reaction conditions can fundamentally change the orientation and arrangement of filler (particularly 2D fillers) within the nanocomposite films, leading to significant control over their final physicochemical, electrical and mechanical properties. In addition, the utility of such matrices in different potential applications will also be presented.

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Nanostructured Bi_2Se_3 Film and Its Glucose Sensing Properties

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Controlling nanostructure is a promising strategy to enhance or modify the performance of materials. Nanostructure has been shown to influence surface charge, band structure, electronic state, and surface area. Specifically, controlling the nanostructure of metal chalcogenides with unique electromagnetic properties can either enhance existing properties or introduce new, desirable characteristics. Bi_2Se_3 has been studied as a promising material for photovoltaic and thermoelectric devices due to its relatively simple electronic structure and n-type characteristics. Notably, Bi_2Se_3 with a rhombohedral crystal structure exhibits topological insulator behavior, where the bulk acts as an insulator while the surface displays metallic properties. In this work, we report the synthesis of nanostructured Bi_2Se_3 films using polymer micelles to impart a uniform pore structure throughout the film. This pore structure significantly increases the surface area of Bi_2Se_3, and we focus on the unique surface conduction properties that arise from it. These surface conduction properties are applied to glucose biosensing, and their effectiveness is demonstrated.

Nickel MOF-74@N-Doped Carbon-Embedded Polymorph Nickel Selenide as A Potential Candidate for Electrode in Asymmetric Supercapacitors

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