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Advances in the Synthesis of Hexagonal Boron Nitride Nanomaterials: Methods and Applications

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Hexagonal boron nitride (h-BN) is a highly promising inorganic compound, attracting significant attention due to its unique combination of electrical insulation, thermal conductivity, light weight, and chemical stability. Over the past decade, the development of h-BN nanostructures has preserved these intrinsic properties while introducing novel nanoscale characteristics. This presentation provides a comprehensive review of the synthesis methods for h-BN nanomaterials across different forms (nanotubes, nanosheets, and porous structures) and their applications in thermal management and water purification. A carbon-free chemical vapor deposition method has been developed for the high-yield, high-purity synthesis of BN nanotubes¹. These nanotubes, with diameters below 10 nm, were fabricated by optimizing the reaction between metal oxides and boron sources. BN nanosheets, with an average thickness of 2-5 nm, were produced via polymerization and crystallization of ammonia borane, using a chemical blowing method². BN nanotubes and nanosheets were incorporated into polymer matrices to create thermally conductive nanocomposites, achieving a 20-fold enhancement in thermal conductivity³. These polymeric nanocomposites are well-suited for heat-dissipation applications in miniaturized, high-speed electronic devices. Additionally, a boraxbased, template-free pyrolysis method was developed to mass-produce cellular monoliths of few-atomic-layer BN, featuring ultra-thin pore walls and uniform mesopores. The porous BN monoliths demonstrated high adsorption capacities for Congo red dye and heavy metals in water purification applications4. Finally, this presentation discusses the major challenges and limitations in the current manufacturing techniques for h-BN nanomaterials and explores future research directions and opportunities⁵.

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Liquid Interface as Delicate Zone for Materials Science: Molecular Machine, Living Cell, and Organic Semiconductor

Ariga Katsuhiko, The University of Tokyo, Japan

Unveiling the Topology-Property Relationship in the Polyethers

Byeong-Su Kim, Yonsei University, South Korea.

Electrically Conductive Nanomaterials-Based Composite Membranes With Electro-Promoted Water Treatment Performance

Xie Quan, Dalian University of Technology, China

Beyond the Lab: Binder Design for Scalable High-Energy Lithium Battery Electrodes

Sang-Young Lee, Yonsei University, South Korea

The Development of Cost-Effective Platforms for Photocatalytic and Non-Photocatalytic Environmental Remediation and Carbon Capture

Ki-Hyun Kim, Hanyang University, South Korea

Ion solvating membranes: Quaternary ammonium-free alternatives to AEM

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Water electrolysis (WE)

Ion solvating membranes (ISM) based on KOH-doped polybenzimidazole (PBI) outperform industry state-of-the art Zirfon diaphragms in terms of conductivity, resistance, hydrogen crossover and electrolysis performance.^[1]

Sulfonation of PBI extends the operational range of ISM from 4-7 M KOH to 0.2-7 M KOH, allowing their use also in anion exchange membrane (AEM) WE.^[2,3,4] Since ISM have no quaternary ammonium groups, they promise a new level of alkaline stability.

Specifically, DBX-crosslinked sulfonated *para*-PBI (5MS-PBI) showed 500 h stable AEMWE performance at 80 °C, 1M KOH.^[3] Further improvements were made by changing chemical crosslinking to thermal curing.^[4] A novel ISM^[5] reached a conductivity of 135 mS/cm in 1M KOH at room temperature. We are not aware of any AEM which has higher conductivity. No alkaline degradation was observed in an ex-situ test (6 months, 80 °C, 1M KOH).

Vanadium Redox Flow Batteries (VRFB)

Several PBI-based membrane systems were investigated. Using thin *meta*-PBI layers supported by sulfonated polystyrene gave access to stable, cheap (<2 US\$/m² materials cost) membranes, and an energy efficiency of 90% at 80 mA/cm². [6] With 23 μ m thick MS-PBI membranes, a world-level energy efficiency of 92% was realized. [7]

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International Conference on Materials Science and Engineering (Materials Oceania 2025)
September 16-19, 2025 | Yonsei University, Seoul, South Korea Revisiting Electrolyte
Thermodynamics Beyond Debye–Hückel Theory Norio Takenaka, a Hinata Koyamada, a
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The development of efficient electrochemical systems for renewable energy storage, conversion, and green hydrogen production is vital for achieving a net-zero society. In these systems, the electrode potential (E) thermodynamically determines the direction and driving force of electron transfer reactions between electrodes and electrolytes. Precise control of E has proven critical in improving the performance of advanced electrochemical devices. For instance, a highly reversible Li plating/stripping was achieved by upshifting E of Li metal, thereby mitigating electrolyte decomposition [1]. Likewise, optimizing the overall potential diagram of a battery system with an organic electrolyte enabled the highly stable operation of earth-abundant SiOx|LiNi0.5Mn1.5O4 batteries with a 4.9 V charge cut-off, accompanied by E shifts of approximately 0.5 V [2]. These remarkable achievements underscore the importance of controlling E via electrolyte engineering for future battery development. Despite its importance, a theoretical framework capable of quantitatively describing E under concentrated conditions remains elusive. The Debye-Hückel theory [3], introduced in 1923, laid the foundation for electrolyte thermodynamics but is restricted to the limit of infinite dilution. Numerous efforts have attempted to generalize this theory, but the explicit treatment of long-range electrostatic interactions in thermally fluctuating, many-body liquid environments has long been impractical. Recent progress in molecular dynamics (MD) simulations now enables direct modeling of such interactions, capturing both spatial and temporal correlations among ions and solvent molecules. In this context, we recently introduced the concept of the liquid Madelung potential [4], which can be used to directly calculate cumulative electrostatic interactions from surrounding solvents and ions in the electrolyte using MD. In this presentation, we present a high-precision computational framework that rigorously determines the total free energies of target ions in electrolytes based on MD simulations. By explicitly incorporating not only electrostatic interactions but also van der Waals interactions and entropy contributions, our approach overcomes the limitations of heuristic approximations and successfully reproduces experimentally observed shifts in E values across all concentration regimes. This advancement offers a comprehensive, physically grounded alternative to the century-old Debye-Hückel theory and establishes a predictive framework for electrolyte thermodynamics in advanced electrochemical systems.

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Recent Developments in Three-Dimensional Junction Bipolar Membranes: Toward Enhanced Water Dissociation Efficiency, Structural Integrity, and Chemical Robustness

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Bipolar membranes (BPMs) have garnered considerable attention for their applicability in green hydrogen production, pH regulation, and the sustainable generation of acids and bases, owing to their intrinsic ability to facilitate water dissociation into H⁺ and OH⁻ ions under an applied electric field. However, their broader deployment is still hindered by significant overpotential requirements and long-term stability issues. In particular, BPMs are prone to dehydration when the water supply rate cannot adequately compensate for the rapid consumption of water molecules during high-current-density operation or prolonged use. This imbalance may lead to interfacial delamination and, ultimately, the deterioration of membrane durability. To address these challenges, the introduction of a three-dimensional (3D) junction—achieved via dual electrospinning—offers a promising design strategy. This interpenetrated junction structure effectively locks the cation and anion exchange layers together, thereby improving interfacial adhesion and enhancing mechanical robustness. Moreover, the 3D configuration substantially enlarges the interfacial area, thereby lowering the energy barrier for water dissociation and reducing the overpotential. Nonetheless, 3D-BPMs are not without limitations. The increased membrane thickness intrinsic to their structure can attenuate the electric field intensity at the junction, which in turn compromises water splitting efficiency. To mitigate this, various catalysts capable of promoting protonation and deprotonation reactions can be embedded within the 3D interface to boost water dissociation kinetics. Given that BPMs operate under conditions involving sharp pH gradients, they are also required to exhibit strong chemical resilience. In this context, ether-free polymers represent a compelling class of materials for BPM fabrication, as they demonstrate superior chemical stability under harsh electrochemical conditions. This presentation will provide a comprehensive overview of the latest strategies for engineering highperformance BPMs, with particular focus on improving structural stability, optimizing water dissociation efficiency, and ensuring chemical durability—three pivotal factors in advancing BPMs toward practical application in electrochemical water splitting systems.

Design of Organic Solar Cells Using Ternary Blends of Semiconducting Polymers

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Designing Nanostructured Catalytic Materials that Steer Selective Electrosynthesis

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Synthesis and Characterization of Nanostructured Carbides for HER

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Due to climate change and limited fossil resources, it is urgent to develop clean and sustainable energy sources. Dihydrogen (H2) is considered as one of the main "energy carriers" of the future.[1] Currently, H2 generation is mostly produced from natural gas, but these processes are hardly environmentally friendly due to large emission of CO2. On the contrary, efficient splitting of water into H2 and oxygen (O2) is a very promising strategy for producing cleaner, safer and more sustainable H2, but sustainable active electrocatalysts are still required for both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). This presentation will summarize our recent works on the synthesis and characterization of molybdenum (Mo) carbides from original routes using transition metal cluster-based precursors or CO2 laser pyrolysis [2-4]. Recently, transition metal carbides demonstrate very interesting electrocatalytic properties, especially Mo carbides for the HER reaction, and they appeared as an interesting alternative to replace critical catalyst materials like platinum or nickel. The resulting carbides were characterized by several complementary techniques (XRD, XPS, BET measurement, SEM, etc.). These innovative modes of synthesis afford nanostructured compounds that are evaluated as catalysts for the HER. [1] Okolie, J.A., et al., Futuristic applications of hydrogen in energy, biorefining, aerospace, pharmaceuticals and metallurgy. Int. J. Hydrogen Energy, 46 8885-8905 (2021). [2] Caroff, T. et al., Facile synthesis and characterization of molybdenum carbides/carbon nanocomposites by laser pyrolysis. Nanomanufacturing 2, 112-123 (2022). [3] Dubois, G. et al., Synthesis and characterization of nanostructured carbide and nitride catalysts by clusters route or laser pyrolysis. J. Jpn. Soc. Powder Powder Metallurgy, 72, S1291-S1297 (2025). [4] Dubois, G. Thesis, « Elaboration de nanomatériaux nitrures et carbures de métaux de transition pour le domaine de l'énergie et de l'environnement ».

Spray-coated Diamond Electrode for Electrolytic Applications

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Conductive boron-doped diamond (BDD) electrodes or diamond electrodes are known to be useful for an extremely durable electrode material for electrolytic applications with a high efficiency, based on their superior properties of wide potential window and physical and chemical stabilities. It has been known that reactive oxidizing species, such as peroxodisulfate, peroxomonosulfate, and hydrogen peroxide, can be generated at a high current efficiency by the electrolysis of concentrated sulfuric acid at diamond electrode. The electrolyzed sulfuric acid containing the reactive oxidizing species exhibits strong oxidizing power, and can be used for mineralization of organic compounds. In this study, we have developed a new method to fabricate a large-sized diamond electrode that can be used for electrolyzed sulfuric acid production by forming a BDD powder (BDDP)/silica composite film via spray coating.

BDDP was prepared by deposition of a BDD layer on the surface of diamond powder with a particle size of 3-6 μm via microwave plasma-assisted chemical vapor deposition. The BDDP was added to tetraethyl orthosilicate/ethanol solution, followed by addition of ultrapure water and nitric acid and stirring to prepare a BDDP/silica sol solution. The BDDP/silica sol solution was spray-coated on a hydrophilic titanium substrate, and after baking at 150 °C for 1 h, a spray-coated diamond electrode consisted of a BDDP/silica layer formed on the substrate was obtained.

10 mL of 50% sulfuric acid was electrolyzed at a constant current density of 20 mA cm⁻² for 90 min at a spray-coated diamond electrode (electrode area: 0.5 cm²). During the electrolysis, the electrode potential was stable around +3 V vs. Ag/AgCl, indicating that no deterioration of the electrode occurred even at highly positive potentials in concentrated sulfuric acid. Current efficiency of reactive oxidizing species formation was calculated to be 41%. These results confirm that the spray-coated diamond electrode can be used for electrolyzed sulfuric acid production. A large-sized spray-coated diamond electrode was also prepared in the same way using a 20×20 cm²-sized titanium substrate. Therefore, the spray coating method is expected to be useful for scaling up of a diamond electrode for sulfuric acid electrolysis.

Integrative Battery Research: From Materials to Intelligent Systems for Future Mobility

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Manipulating Nanostructure-Evolution under Dynamic Conditions for Advanced Electrochemical Devices

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With the presence of complicated multi-physics fields, the evolution of nanostructures and the electrochemical process often exhibit unpredictable and chaotic characteristic. As a result, 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. The classical Self-organization Theory says that proper energy and informational flows can trigger local interactions between elements in a system and thus incur emergence of regular patterns with resilience and adaptation characteristics. 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 technical transfer progress of some of the techniques [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 with unprecedented performance.

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Printed Porous Composite Layers for Flexible Sensor

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Multilayer Nanoporous Graphene Membrane for Ultrafast Organic Solvent Nanofiltration

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Graphene-based materials have potentially been utilized for organic solvent nanofiltration (OSN) membranes due to their interlayer structure and excellent mechanical and chemical stability, which enables precise molecular sieving in harsh conditions, e.g., in toxic organic solvents. Pore generation on graphene techniques has been applied to enhance the solvent flux because the activated nanopores with an appropriate size can accelerate the transport of solvent molecules while maintaining high selectivity. In this talk, several post-pore activation methods for nanoporous graphene will be discussed with applications as high-performance OSN membranes. The nanopores could be generated on the basal plane of graphene by the thermal or chemical treatment of GO. In particular, sp² carbon domains were additionally recovered from amorphous sp³ carbon structures through microwave-assisted reduction. The resulting multilayer nanoporous graphene membranes are capable of ultrafast organic solvent filtration with precise molecular sieving. Furthermore, the membranes were feasible for the separation of multiple mixed solutes in various organic solvents. I will also discuss the solvent flow mechanism through the porous multilayer graphene, particularly focusing on the critical pore size and interlayer spacing for ultrafast solvent flow.

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Stabilization of Overloaded Pharmaceutical Glass Using Mesoporous Silica Particles

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Although crystalline drugs are usually used for solid pharmaceutical products, amorphous state is sometimes employed because of its higher solubility. The amorphous state of the drug during long-term storage must be maintained for exerting its advantage, for which excipients are used for stabilization. Mesoporous silica is one of the promising excipients, as entrapped molecules in pores are stabilized against crystallization. However, a large amount of silica materials is required for the stabilization based on this idea, which is not favored from a viewpoint of formulation volume. On the other hand, the stabilization effect is unclear if guest molecules are overloaded, that is, a larger amount of guest molecules are mixed than pore capacity of the carrier.

In our study, celecoxib (CEL) glass was mixed with mesoporous silica microparticles having different pore sizes, 2.5 nm and 21 nm, using grinding followed by heating above melting temperature of CEL. Differential scanning calorimetry (DSC) was used to discriminate molecular state of CEL glass into three: free, intermediate, and rigid fractions. The free fraction exhibited cold crystallization during DSC heating, which was understood to have almost the same properties with bulk molecules. The rigid fraction did not show either glass transition or cold crystallization, which was assumed to be stabilized by interactions with the silica surface. The remaining provided the glass transition behavior without any tendency of cold crystallization during the DSC heating, which is defined as an intermediate fraction. Broadband dielectric spectroscopy (BDS) was used for evaluating molecular mobility of each fraction. Intermediate and free fractions had similar mobility, whereas that of the rigid fraction depended on pore size. Accelerated and suppressed molecular mobility were observed for the molecules entrapped in 21 and 2.5 nm-pores, respectively. The pore size of 21 nm is much larger than the cooperatively rearranging region (CRR) of the CEL glass, whereas 2.5 nm was comparable to that. When the pore size was larger than that of the CRR, most of the loaded CEL molecules behaved as an intermediate fraction, probably because the molecules were exchangeable inside and outside the pore. On the other hand, the exchange seemed to be slow when the pore size was comparable or smaller than that of the CRR, leaving a large amount of free fraction. Isothermal crystallization study of overloaded CEL glass revealed that the CEL glass mixed with the silica particles with the large pores exhibited slower crystallization relative to the free CEL, whereas accelerated crystallization was observed for the CEL mixed with a small amount of the silica particle with small pores. By increasing amount of silica particles, stabilization of CEL glass was found for both silica particles; however, the silica with the larger pore showed better stabilization effect, which was explained in terms of the easiness of exchange of inside/outside molecules. This finding proved stabilization effect of mesoporous materials is effective not only for the entrapped molecules but also for overloaded ones, if the pore size is large enough for the exchange.

Porous Silicon Nanoparticles for Overcoming Brain-related Diseases

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Nanoscale structured materials possess unique optical, electronic, mechanical, and biological properties. In the biomedical field, various types of nanomaterials have been introduced and garnered attention in nanomedicine because they have the potential to overcome the severe drawbacks of pharmacologically active agents, including lack of water solubility, biological stability, and ineffectiveness of in vivo targeting. Many nanosized particle systems have been developed as delivery vehicles based on organic (liposomes, protein or peptide aggregates, polymers, etc.) and inorganic (quantum dots, metal nanoparticles, nanotubes, silica nanoparticles, etc.) composites. Among them, porous silicon nanoparticles (pSiNPs) have attracted attention as a promising drug delivery system (DDS) platform owing to their remarkable features: (i) a high loading yield of the substrate (drugs, peptides, DNA/RNA, proteins, antibodies) and maintenance of the bioactivity of the encapsulated substrate, (ii) targeted delivery (cells, organs, disease sites) with the incorporation of targeting moiety (peptides, sugars, proteins, nucleic acids, etc.), (iii) in vivo biodegradation and fast clearance of non-toxic side-product (silicic acid, Si(OH)4), (iv) high biocompatibility, and (v) multi-functional platforms (bio-imaging, theragnostic). In this talk, the speaker will present recent research on a drug delivery system using porous silicon nanoparticles for brain-related diseases, such as glioblastoma (GBM) and Alzheimer's disease (AD).

Synthesis of Two-dimensional Metal-organic Frameworks

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Two-dimensional metal-organic frameworks (2D MOFs), a class of ultrathin, porous crystalline materials formed by the coordination of organic ligands with metal nodes, have demonstrated remarkable potential in energy storage/conversion, catalysis, and sensing due to their abundant exposed active sites, short electrolyte diffusion pathways, and good electrical conductivity. However, the MOFs comprise organic ligands and metal nodes, which connect each other and extend infinitely in three-dimensional space, resulting in bulk products. The challenge is maintaining two-dimensional epitaxial growth while suppressing spontaneous three-dimensional self-assembly to achieve 2D MOFs. To address this, we tried to synthesize two 2D MOF materials via recrystallization and competitive coordination strategies, then investigated their electrochemical energy storage behavior. Electrochemical evaluations demonstrated exceptional performance with a high specific capacitance. This work highlights a modulator-free, sustainable approach for MOF nanoarchitecturing, with implications for advanced energy storage materials.

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Transformation of the Phase and Shape of Transition Metal Dichalcogenides via Molecular Surface Treatments

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Transition metal dichalcogenides (TMDCs) are two-dimensional materials that have attracted significant attention from both scientific and engineering perspectives. Their appeal stems from their unusual transport and optical properties, as well as their potential for enabling further downscaling of device structures. These atomically thin layered materials also exhibit intriguing physicochemical properties, including phase transitions between semiconducting, metallic, superconducting, and topological states. Moreover, the stacking structure of these thin layers significantly influences their properties. For example, monolayer and bilayer forms of MoS₂ differ in their electronic band structures: monolayer MoS₂ has a direct band gap, while bilayer MoS₂ exhibits an indirect band gap. Recently, the stacking angle between layers in bilayer structures has also garnered interest, as it can further modify material properties. In this presentation, I will introduce our recent research on molecular treatments for inducing phase transformations, as well as solution-based methods for forming bilayer structures. One of the notable phases in TMDCs is the 1T' phase, which is known to exhibit semimetallic behavior and topologically protected properties. In our work, we discovered a method to convert the semiconducting 1H phase to the 1T' phase in monolayer MoS₂. This conversion is initiated by oxidative treatment using ozone molecules, and is further facilitated and stabilized by the enwrapment of an organic polymer. Notably, the 1T' phase cannot be maintained without the presence of this polymer. Another topic of our research focuses on generating bilayer structures by bending monolayer MoS₂ . We developed a solution-based process in which micron-scale droplets are formed in an organic solution. These droplets induce bending of the monolayer on the substrate, resulting in the formation of numerous bilayer fragments. In the presentation, I will explain the details of both approaches and discuss the mechanisms involved in these transformations. [Ref] K. Matsuyama, et al., Journal of the American Chemical Society, 2025, 147, 16729-16374.

Lyotropic Liquid Crystalline Phases for Designing Porous Electrodes for Various Applications

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Metal salts and non-volatile acids can form lyotropic liquid crystalline mesophases at very high salt and acid concentrations. ^{1,2} These salt–surfactant and salt–acid–surfactant mesophases can be coated onto various substrates with controllable thickness, and their subsequent calcination yields mesoporous thin films or electrodes. ^{3,4} These electrodes exhibit excellent electrocatalytic performance in the oxygen evolution reaction (OER) and show high capacitance.

This presentation will focus on mesophases formed using two-salt systems—comprising alkaline earth and transition metal salts—with 10-lauryl ether, as well as ternary systems involving lithium salts, transition metal salts, H_3PO_4 or $H_4P_2O_7$, and the block copolymer P123. These systems are used to fabricate thin-film electrodes of porous MgM₂O₄, CaM₂O₄, LiMPO₄, and M₂P₂O₇.

All resulting electrodes demonstrate strong performance in the OER and exhibit good capacitance in alkaline media.³⁻⁵ However, these electrodes undergo surface transformations during operation, forming active metal hydroxide layers. This transformation is complete in lithium metal phosphate and metal pyrophosphate systems and partial in metal oxide systems. The underlying mechanisms driving these transformations will be discussed in this talk.

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Mesoporous Clay Structures for Heterogeneous Catalyst and Support Material

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Clay, which has a multilayer structure, is a silica-based material that exists relatively abundantly on Earth. However, clays that exist in nature generally exist in a mixed form with various other structures and components, so in order to use them for specific purposes, reactions in an imprecise form or the inconvenience of having to go through multiple steps are required. In addition, the multilayer structure of clay has fine gaps in the order of angstroms, so it has an adsorption capacity, but the layers are attached by relatively strong electrostatic forces such as hydrogen bonds, so it has only limited applications according to the pore size. Even if a mechanical or chemical exfoliation process is performed, the size of the effect according to the additional process may not be constant each time. In this study, we introduce a mesoporous clay structure that was developed for chemical mass production rather than a clay structure obtained from nature. We introduce a synthesis method of nickel phyllosilicate with 0D spherical particles and 1D rod-shaped mesopores, and present its physicochemical properties and examples of catalytic applications.

Deciphering Functional Emergence in Advanced Superconducting Wires through Deep Learning Segmentation of 3D Microstructures

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The functional performance of advanced ceramic materials is closely linked to their complex microstructures. With the recent advances in AI technologies, microstructural information is increasingly utilized for multifaceted prediction and optimization of material performance. However, accurate quantification of such microstructures remains a significant challenge, particularly in polycrystalline ceramics composed of grains with varying sizes, shapes, and orientations. Magnesium diboride (MgB₂) is a promising superconducting material due to its relatively high critical temperature, suitable for applications at cryocooler and liquid hydrogen temperatures. Long-length MgB2 wires are typically fabricated using the powder-in-tube (PIT) method. Recent research has focused on the development of multifilamentary wires for high-field magnet applications [1]. However, a notable challenge arises in that increasing the number of filaments often leads to degradation of the critical current density. To address this, we employed a semantic segmentation approach based on deep learning—originally developed for medical image processing [2] and previously demonstrated its applicability in identifying constituent phases in polycrystalline materials with complex microstructures [3]. In this study, we applied this method to quantify and analyze the 3D filament architecture of a MgB₂ multifilamentary superconducting wire using 3D scanning electron microscopy (3D-SEM). The sample under investigation, currently under development [4], comprises 51 superconducting filaments (~10 µm in diameter) arranged in a circular geometry. 3D-SEM observations were performed on a representative region containing multiple filaments. Secondary electron images and manually segmented labels were used as training and testing datasets for a deep learning model. Based on 1,232 acquired images, semantic segmentation followed by 3D reconstruction enabled successful quantification and visualization of the internal filament structure. This approach provides a powerful tool for understanding the microstructure-function relationship in advanced superconducting wires.

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Computational Design of Electrochemical Energy Conversion Materials Using Firstprinciples Calculations and Machine Learning Techniques

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The first step to design highly active nanomaterials for renewable energy applications under electrochemical media is clear understanding of structure—property-performance correlation. For example, solid-stat electrolytes play key role for safer operation of lithium-ion batteries, however, its undesirably low ionic conductivities have delayed commercial applications. Nanoscale electrocatalysts are key components for renewable energy conversion reactions, but till now none satisfy the three criteria of activity, selectivity and stability in active liquid media.

This presentation demonstrates a self-driving computational strategy to empower efficient and precise screening exploration of unknown candidates and exploitation of known materials, which are highly functional for energy storage and conversion reactions in electrochemical systems. Combined with first-principles DFT calculations and machine learning techniques with advanced algorithms we show that rigorous working principles for experimentally discovered nanomaterials can be elucidated. Moreover, design principles for even empowering higher performance are proposed. Most interestingly, several candidates are suggested, which can get over long-standing challenges to the nanomaterials applied to energy storage and conversion. As example, we show single atom catalysts, which are bifunctionally very active (oxygen reduction and oxygen evolution reactions) very active and allow the performance tunability according to target purpose. In addition, design principles how to synthesize a stable Li-argyrodite with high energy density for long electrochemical cyclic lives.

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Multi-scale Modeling and Inverse Design of Catalytic Substrates for Isothermal Segregation Growth of Two-dimensional Materials

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Abstract

For a long time, the controllable synthesis of large-area, high-quality, multilayer two-dimensional materials has remained a core challenge in the field of two-dimensional materials. Traditional methods such as chemical vapor deposition and molecular beam epitaxy exhibit significant limitations in precisely controlling layer numbers, reducing defect density, and ensuring structural uniformity, which severely restricts the large-scale applications of twodimensional materials. The recently emerged isothermal segregation method ingeniously utilizes the enrichment phenomenon of solute atoms on alloy substrate surfaces to achieve controllable growth of two-dimensional materials under constant temperature conditions. This method offers remarkable advantages: first, it eliminates the need for complex temperature gradient control, greatly simplifying the synthesis process; second, precise control of twodimensional material layer numbers can be achieved through accurate adjustment of substrate alloy composition ratios; third, the growth process under isothermal conditions is closer to thermodynamic equilibrium, favoring the formation of higher-quality and more uniform two-dimensional structures. Previous studies have demonstrated that the isothermal segregation method has successfully achieved the synthesis of various two-dimensional material systems including graphene, h-BN, and transition metal dichalcogenides. However, designing optimal segregation substrates for different two-dimensional material systems still faces significant challenges, urgently requiring in-depth revelation of the structure-activity relationship between atomic segregation behavior and alloy substrates, which highlights the crucial role of theoretical simulation and computational design in this field.

Based on first-principles calculations, this study systematically investigates the decomposition mechanism of carbon source molecules on CuNi alloy substrates, the migration behavior of carbon atoms within substrates, and the nucleation and growth process of graphene on substrate surfaces, revealing the precise regulatory effect of alloy composition ratios on graphene nucleation density and carbon atom migration rates, thereby influencing graphene crystal quality. Additionally, we studied the growth mechanism of h-BN on N2 and FeB substrates, clarifying the crucial roles of B atom defects and N atom migration in h-BN formation. Building upon these studies, we further constructed a theoretical model for isothermal segregation growth of two-dimensional materials and utilized this model to screen PtNi and CuNi alloy substrate systems suitable for graphene isothermal segregation growth, revealing the intrinsic correlation between two-dimensional material segregation behavior and alloy composition as well as crystal facet orientation. Furthermore, through machine learning force field-accelerated molecular dynamics simulations, we validated the accurate prediction of this theoretical model for graphene growth kinetics, with simulation results highly consistent with first-principles calculations and further confirmed by experimental verification of the model's effectiveness. This model is not only applicable to graphene material systems but also provides a universal theoretical framework for isothermal segregation growth of other two-dimensional materials, establishing a complete research paradigm from theoretical design to experimental validation, and offering novel theoretical guidance and important technical support for achieving large-scale synthesis of high-quality, layercontrollable two-dimensional materials.

Analytical modeling and mechanical behaviors of crosslinked graphene layers

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This study presents a comprehensive investigation of the mechanical properties of layered graphene-based nanomaterials enhanced by multimodal crosslinking strategies, employing a nonlocal elasticity framework. Using an analytically derived deformable tension-shear model that considers the nonlocal continuum mechanics, we examine how elastic deformation and nanoscale interactions influence the mechanical performance of graphene-based materials, including papers, fibers, and films. Traditional tension-shear models often neglect critical elastic effects that arise at the nanoscale, especially in confined layered systems where surface forces and interfacial bonding dominate mechanical behavior. To address this issue, we adopt a nonlocal elasticity approach to more accurately describe load transfer across functionalized graphene sheets connected by engineered crosslinking networks. These crosslinks include a synergistic combination of long, strong covalent bonds and short, reversible (self-healing) interactions. The introduction of these multimodal crosslinks enhances both strength and toughness by enabling efficient stress redistribution and energy dissipation during mechanical loading. Our theoretical analysis identifies two primary failure mechanisms: (i) fracture of the graphene layers and (ii) rupture of the interlayer crosslinks. Atomistic simulations support these theoretical predictions, revealing that reversible short crosslinks contribute significantly to toughness through their ability to rupture and reform under mechanical stress. Simultaneously, the presence of longer, permanent crosslinks provides necessary structural integrity and stiffness, preventing catastrophic failure. Together, this multimodal crosslinking architecture enables superior mechanical performance by promoting cooperative deformation mechanisms across multiple length scales. The model further demonstrates that the mechanical behavior of these materials is highly sensitive to several structural parameters, including the size of the graphene flakes, the density, type, and spatial distribution of the crosslinks, and the interlayer distance. Smaller flakes with dense and strategically arranged crosslinking sites yield more uniform stress distributions, enhancing both strength and ductility. Furthermore, the interplay between reversible and permanent crosslinks can be tailored to achieve application-specific performance—ranging from highly resilient to highly rigid material systems. These tunable characteristics make layered graphene-based nanomaterials ideal candidates for multifunctional material systems. Furthermore, we systematically analyze how key structural parameters-including graphene flake size, crosslink strength, and interlayer spacing—govern the overall mechanical performance. The result shows that stress transfer process is a fundamental concept in structural mechanics, especially for layered materials or composites containing layered materials. Effective stress transfer in layered graphene-based nanomaterials is key to achieving high mechanical stiffness and strength. Therefore, understanding and optimizing stress transfer mechanisms are essential to improve performance and ensure reliability. These findings open new avenues for designing next-generation macroscopic materials from low-dimensional building blocks. The ability to tune interfacial mechanics via rational crosslinking strategies provides a powerful tool for optimizing the performance of graphene-based materials in diverse engineering applications, including flexible electronics, smart sensors, structural composites, energy-absorbing fabrics, and biomedical scaffolds. In summary, this study provides fundamental insights into the mechanics of crosslinked layered nanomaterials. Theoretical simulations and analytical results demonstrate that multimodal crosslinks synergistically transfer tensile loads, thereby enhancing strength. Meanwhile, reversible rupture and the formation of healable crosslinks improve toughness.

Ultra-flexible skin-compatible organic optoelectronics

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Ultra-conformable organic optoelectronic devices are transforming biomedical applications and wearable technology, shaping the next phase of the Internet of Things. The inherent mechanical compliance of organic materials, coupled with their scalable and cost-efficient fabrication, has propelled advancements in state-of-the-art sensors and energy harvesting systems. Yet, balancing electronic performance with mechanical resilience remains a significant hurdle. This presentation highlights recent progress and persistent challenges in organic ultra-flexible electronics. We delve into material innovations and structural design strategies that have facilitated the creation of highly adaptable devices for direct skin integration. Our research presents approaches to maintaining optical and electrical stability under deformation, ensuring reliable function in dynamic conditions. Beyond material and structural advancements, these devices hold promise for a wide range of applications, including continuous physiological monitoring, motion detection for AR/VR, and next-generation medical systems. By sharing our insights, we seek to drive further exploration into wearable electronics that naturally conform to the human body. Ongoing progress in this domain is set to enhance quality of life while expanding the role of intelligent, interconnected technologies in daily routines.

Metallurgy Revised

John Campbell, University of Birmingham, UK

Incremental Forming of Tailor-Welded Sheet of AA1050 Aluminum with Dissimilar Thickness Made by Bobbin Tool Friction Stir Welding

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Tailor-welded sheets are widely used to reduce the weight of transportation equipment. During the welding process, not only different materials but also sheets with different thicknesses are joined. For aluminum alloy sheets, friction stir welding is a commonly adopted method. Meanwhile, the growing demand for rapid manufacturing of sheet metal products has led to increasing use of incremental forming—a flexible forming technique similar to 3D printing that requires only a simple rod-shaped tool and does not require dies. In this study, tailor-welded aluminum sheets were formed into a cup shape using incremental forming. The weldability and formability conditions were investigated.

A1050-O pure aluminum sheets of 1.5 mm and 2.0 mm thickness were used as test materials. These sheets were welded in three different thickness alignments using a custom-designed bobbin-tool friction stir welding technique. The initial tool feed rate during lead-in was set to 20 mm/min, which was maintained until a stable weld was achieved. After the first 20 mm of welding, the process was continued at various tool feed rates ranging from 20 to 400 mm/min. The tool rotation speed was fixed at 1000 rpm, and the tool gap was kept at 1.4 mm. After welding, cross-sectional observations were conducted and grain sizes were measured. Next, the tailor-welded sheets were formed into a truncated pyramid shape using incremental forming. The side wall angle was varied, and formability was evaluated based on the minimum formable angle. Fracture positions and their causes were analyzed using strain distribution.

The grain size in the stir zone of specimens aligned at the center of the sheet thickness was found to be smaller. All tailor-welded sheets that fractured after forming showed cracks at the weld joints. Sheets with welds positioned at the center of the thickness direction demonstrated improved forming limits compared to other alignment methods. However, during leftward forming of sheets with center weld position and a 2 mm advancing-side sheet, the forming accuracy was the lowest.

Synthesis and Structural Characterization of Phosphine Ligands for Pd-catalyzed Carbonylations

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Pd-catalyzed carbonylation (such as alkoxycarbonylation, aminocarbonylation and hydroxycarbonylation) of alkenes/alkynes, has emerged as a valuable and green methodology for synthesis of carbonylated compounds (like esters, amide, and carboxylic acids etc.), advantageous with 100% atom economy. Therein, the phosphines with different stereoelectronic properties play pivotal role in tuning the performance of the involved Pd-catalysts, in terms of activity, chemo-/regio-selectivity, and stability. Hence, the design and synthesis of novel phosphine ligands is always a highly demanded task to improve the carbonylation efficiency. We focus our effort on developing the phosphine ligands with different steric effect and electronic effect. The structural features the as-synthesized phosphine ligands as well as the corresponding Pd-complexes were characterized by single crystal X-ray crystallography. And the co-relationship between the ligand structures/compositions and performance the Pd-catalysts for carbonylation of alkenes/alkynes were investigated [1-3].

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Advanced Materials for Roadway Infrastructure Renewal: The Role of Composite Materials in Sustainable and Resilient Rehabilitation Strategies

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Advanced Functional Materials and Technologies for Additive Manufacturing of 5G/6G applications

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The next generation of 5G/6G wireless networks based on RF and mm-Wave devices promise to bringing fast, stable and low latency connectivity at low cost. However, RF and mm-Wave telecommunications brings with it new challenges as these wavelengths travel short distances, are ineffective at penetrating walls and are more susceptible to loss due to environmental factors. The workaround to these drawbacks has been to develop 5G/6G networks that function off of small networking cells that use arrays of antennas in small geographical areas. These small cell networks transmit data using highly directional waves using large numbers of antenna arrays and lenses to ensure continuous and rapid transmission of signal. Dielectric materials are utilized in many parts of 5G/6G devices (antennas, filters, power dividers, lenses, radomes, polarizer, foam/substrates). In order to meet the stringent requirements of future 5G/6G networks, the development of low-loss tangent (dissipation factor) dielectric materials is key in high-frequency and high-speed environments. Many of these devices could have enhanced performances if the dielectric materials could be designed with complex geometries. For instance, Luneburg lenses, components that focus RF and mm waves are used to improve the gain of signal transmission. These can be manufactured as complex lattices with gradients in their porosity. Similarly, power dividers and dielectric resonator antennas, can be designed with geometric complexity to enhance their performance. Components with complex 3D geometries cannot easily and cost effectively be produced using traditional manufacturing methods. In general, RF and mm-Wave dielectric components are fabricated using traditional manufacturing methods with organic and inorganic low loss materials available in the market. Most of these materials have not been developed as 3D printable materials. 3D printing provides a means to manufacture low-cost lenses/antennas with complex 3D designs. In particular, vat polymerization 3D printing is unique in its ability to fabricate 3D objects from photoresins at a high speed and high-resolution print using diverse types of materials. The 3D printing methods such as stereolithography (SLA), digital light processing (DLP), and volumetric additive manufacturing (VAM) are particularly attractive for manufacturing RF and mm-Wave components as the printing platform prints to higher print quality, which will ensure higher performance in the device. Therefore, the development of new 3D printable low-loss dielectric photoresins is highly desirable in order to fabricate the high resolution, light-weight, complex, miniaturized and high-performance (gain, beamforming etc.) mm-wave devices for 5G/6G technologies. In this talk, I will be presenting the development of highly customizable low-loss dielectric materials compatible with vat polymerizable 3D printing through the selection of monomers, crosslinkers and fillers. The materials properties can be tuned at the molecular level (formulation) and at the microscale (through printing parameters) to obtain optimized 3D printed lenses/antennas and further their performance in mm-Wave region.

Title of Paper Here, Title Case, in Bold, Centered 12 Point Type

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The Role of Natural Fibers in High-Strength and sustainable Composites. Thamer Alomayri **

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Abstract: Natural fibre-reinforced concrete is gaining popularity in the building sector as a more environmentally friendly alternative to synthetic reinforcements. Bamboo, hemp, coconut coir, and jute are environmentally friendly since they are renewable, biodegradable, and made from agricultural waste. These fibers improve the mechanical qualities of concrete, such as toughness, tensile strength, fracture resistance, and durability, by preventing cracks from spreading and increasing the material's ability to absorb energy. They improve the sustainability of concrete by reducing its environmental effect and promoting waste-to-resource operations. Despite these benefits, concerns about the fibres' compatibility with the cement matrix persist. These issues include the fibers' capacity to absorb water, as well as their natural and chemical deterioration over time.

Design of Stable and Highly Efficient Conjugated Polymer/2D Nanosheet P-N Heterojunction Composites for Hydrogen Evolution Reactions

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We successfully developed a two-dimensional nanocomposite material with an organic-inorganic P-N heterojunction interface to serve as an efficient electrocatalyst for the hydrogen evolution reaction (HER) in acidic aqueous environments. Organic polyaniline (PANI) and inorganic exfoliated tungsten disulfide (WS2) nanosheets are P-type and N-type semiconductors, respectively, and their combination efficiently facilitates formation of a P-N heterojunction that significantly enhances charge transfer from PANI to WS2 during HER catalysis. Herein, by combining sodium ion-functionalized chitosan (Na-CMC)-assisted WS2 exfoliation, electrochemical polymerization of PANI, and subsequent electroactivation treatment on a highly conductive nickel foam (NF) substrate, we efficiently obtained a Na-CMC/WS₂/PANI/NF electrode with outstanding electrocatalytic performance. NaCMC/WS2/PANI/NF electrode demonstrated superior electrocatalytic hydrogen evolution performance in acidic electrolytes compared to a commercial precious metal Pt/C catalyst, with a lower overpotential, reduced resistance, and a Tafel slope of 35.2 mV/dec. Under prolonged operation at a current density of 100 mA/cm² and repeated cyclic voltammetry scans, the Na-CMC/WS₂/PANI/NF electrode demonstrated remarkable long-term catalytic activity and structural stability, indicating its potential as a durable and efficient hydrogen production electrocatalyst. This study provides new insight for development of organic-inorganic non-precious metal electrocatalysts with P-N heterojunction interfaces for various energy sectors.

Magneto-dielectric effect in corundum-type oxide

The corundum type M4A2O9 [M = Mn, Fe, Co, Ni & A = Nb, Ta] ceramic materials have renewed research interest in last few decades because of their distinct magnetoelectric properties. We have thoroughly studied the structure, magnetic and magneto-dielectric properties of Co4NbTaO9 along with the isotypic Co4Nb2O9, Co4Nb1.5Ta0.5O9 and Co3NiNb2O9 phases, which are noncollinear antiferromagnet with trigonal structure. The synthesis of ceramic samples was carried out by solid state reaction method. Magnetic studies reveal the transition temperature decreases with Ta substitution, whereas it increases with Ni substitution. In the absence of external magnetic fields, no dielectric anomaly is noticed below the magnetic transition temperature. However, prominent dielectric peak appears under external magnetic fields and the peak magnitude increases with increasing field strengths, depicting magneto-dielectric and magnetoelectric phenomena. We describe the magnetic field induced dielectric effect due to the spin-flop magnetic transition.

Polyisoprene-Coated Silica for Non-Black Rubber: Enhancing Processing, Mechanical, and Barrier Properties

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This study presents a surface-engineering approach to improve the processing characteristics, mechanical strength, and gas barrier performance of natural rubber materials used as inner rubber tubes. This improvement is achieved by incorporating silica functionalized via admicellar polymerization. The resulting polyisoprene-coated silica exhibited optimized properties, including a 14.17% polymer coating, low bulk density (0.26 g/cm³), and high absolute density (1.62 g/cm³), promoting enhanced compatibility with the natural rubber matrix.

Inner rubber tube-based compounds with a green color pigment and 30 phr of the coated silica demonstrated significantly improved processability. This was indicated by lower Mooney viscosity and shorter cure times compared to those formulated with conventional fillers like bare silica or carbon black. Mechanical evaluations revealed notable enhancements in tensile strength, elongation at break, tear resistance, and 300% modulus. Moreover, gas permeability testing confirmed that the coated silica substantially improved barrier properties, outperforming traditional carbon black-based rubber. The non-black appearance and excellent pigment compatibility of the coated silica also support its use in customized, colored rubber products. These results highlight polyisoprene-coated silica as a high-performance, sustainable alternative filler for next-generation rubber and advanced elastomeric products.

Keywords: Functionalized silica; Admicellar polymerization, Natural rubber compound, Processability; Properties

EVALUATING THE IMPACT OF MANUFACTURING PARAMETERS ON PROPERTIES OF SUNN HEMP BIO-COMPOSITES

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Abstract:

Sunn hemp fibre-reinforced bio-composites offers a new type of sustainable materials and detailed understanding on how the different forms influence their mechanical properties is important. This study investigates mechanical behaviour of sunn hemp bio-composites with different fibre forms using a response surface-based D-optimal experimental design for comprehensive analysis and optimisation of manufacturing parameters. Four control factors—temperature, pressure, time, and fibre form—were combined to evaluate flexural, tensile, and interlaminar shear strengths. Sunn hemp fibre composite boards were manufactured using bio-epoxy resin in compression moulding. Bast fibre form yielded the highest mechanical properties, with tensile, flexural, shear strength, and stiffness values 71.3 MPa, 95.1 MPa, 9.0 MPa and 8185.4 MPa. These properties are at least 35% higher than hurd and hurd-bast composites. Optimal conditions were obtained at 80°C moulding temperature, 6 MPa moulding pressure, and 15 minutes moulding time, achieving a desirability of 75%. Quadratic models developed using response surface methodology (RSM) predict tensile, flexural, and interlaminar shear strengths with confidence levels of 92%, 93%, and 90%, respectively.

Data-driven Investigation of Lattice Parameter Evolution in Fe-based Superconductors

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Iron-based superconductors, especially K-doped BaFe₂As₂ (K-Ba122), are promising for high-magnetic field applications such as in fusion reactors, particle accelerators, and high-resolution MRI devices[1][2]. Yet, the development is hindered by FeAs and Ba-O grain boundary wetting phases that limit the superconducting current flow^{[3][4][5]}. Although the mechanisms behind FeAs and Ba-O formation remain poorly understood^[5], our previous work shows that yttrium addition effectively suppressed FeAs phases^[6], accompanied by systematic changes in lattice parameters. Herein, we investigate the structural evolution of Y-doped K-Ba122 bulks by integrating domain knowledge with data-driven analysis. We distinguish the contribution of high energy milling induced lattice distortions^[7] from those of yttrium doping by synthesizing both BaFe₂As₂ and Ba_{1-x}Y_xFe₂As₂. The samples were prepared by mechanical alloying of elemental metals through high energy milling and consolidation of precursor powders via Spark Plasma Sintering (SPS)^[8]. The material characterizations included X-ray diffraction analysis, microstructural observation, and superconducting properties measurements. Experimental data consisting of SPS conditions (temperature, dwell time, and applied pressure) and yttrium concentration were analyzed using interpretable AI models to assess their influence on lattice parameters (a- and c-axis lengths). To address multivariate and non-linear interactions, we benchmark regression models and feature attribution techniques to identify key synthesis parameters. Our approach aims to validate whether the lattice distortion trend is truly systematic and chemically meaningful, guided by statistical rigor and physical insight. This work highlights the potential of AI in materials design, particularly for Fe-based superconductors^[9], where data-driven interpretability remains underexplored.

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Development of Robust and Environmentally-Freindly Photocatalysts and Photoelectrocatalysts for Organic Removal and Green Hydrogen Production

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Applications of photocatalysis can provide us proper solutions for air purification, water purification, clean energy production, and surface self-cleaning that we have faced with. In particular, it is very important global issues to improve industrial applications of novel photocatalysis to tackle with global climate change or clean/green energy production or carbon neutrality. Real applications of conventional TiO₂ photocatalysis have been limited by high energy consumption like ultraviolet required for generation of photo-generated charge carriers and their easy recombination resulting in decreased their photocatalytic performance. Another significant drawbacks of conventional TiO₂ photocatalysts for improving industrial applications originate from their limited surface area availability for surface-photo reactions and easy loss of photocatalyst materials during reactions and catalyst handling procedures due to their low coating efficiency on substrate surfaces. The current presentation deals with developed ideas or summary to overcome limitations or drawbacks of conventional TiO2 photocatalysis and then also aims to provides some strategies to improve real applications of novel photocatalysts which are active under visible light or sun light irradiation rather than ultraviolet and also show improved photocatalytic activities and durability. The current presentation include some recent techniques or strategies to develop robust and environmentally-friendly photocatalysts or photoelectrocatalysts, including metal or non-metal doping, morphological or structural change, building heterojunction, coating improvement, surface passivation, combination of photocatalysis with photoelectrochemical or photovolatic techniques, etc.

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Entropy-driven derivative organic coverage designs on Ni-rich layered cathodes in lithium-ion battery

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Ni-rich layered cathodes have a high practical capacity (>200 mAh·g⁻¹) and tapped density (>3.6 mg·cm⁻²), thus attracting wide attention in large applications such as electric vehicles and energy storage. However, high surface reactivity of these cathodes promotes the decomposition of carbonates solvents, which contributes to the growth of the cathode–electrolyte interphase (CEI) as well as rapid fading of the battery's capacity during long-term cycle. Carbonates are favorable for deprotonation reaction by the oxygen atom in the Ni-rich layered cathode and further in the formation of the CEI. Previously, we developed a cis formed (linear structure) oligomer organic coverage that use to prevent the deprotonation of ethylene carbonate (EC) on NCM811. The operando FTIR measurement observed the EC is step-by-step deprotonated and transformed to two final products, vinylene carbonate (VC) and carbonate oligomer. The VC then crossovers to anode as solid electrolyte phase formation as well as the carbonate oligomer deposits on cathode surface as cathode electrolyte interphase [1]. In this study, a new organic coverage has been developed, an entropy-driven derivative compound (o-CI) that consists of positive entropy value (28.5 J/ mol K) is used to cover on NCM811. Research results demonstrate the positive entropy design is able to deprotonate two protons from EC simultaneously rather than the step-by-step deprotonation. The benefits of direct and complete deprotonation of EC are the formation of VC and significant eliminates carbonate oligomers. The VC is an electrolyte additive which induces SEI formation on anode side spontaneously that enhances ionic diffusivity. Furthermore, less carbonate oligomers deposits on cathode also decrease the impedance of battery. Compare with the compound (m-CI) with a negative entropy value (-10.5 J/mol K), our result [2] shows the cycle performance of m-CI is not significant improved but o-CI show promising result that may useful for further development in Ni-rich layered cathodes.

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International Conference on Materials Science and Engineering (Materials Oceania 2025) September 16-19, 2025 | Yonsei University, Seoul, South Korea High performance nano-bulk Si-Ge thermoelectric materials

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Thermoelectric power generation is regarded as one of the key technologies for a sustainable, lowenergyconsuming society. The performance of thermoelectric generators is known to be an increasing function of the dimensionless figure of merit $ZT = S^2 \sigma T \kappa^{-1}$, where S, σ , and κ^{-1} represent the Seebeck coefficient, electrical conductivity, and thermal conductivity, respectively. The highest ZT ever reported for bulk materials is less than 3.2, and this value is insufficient to encourage the widespread use of thermoelectric generators in practical applications. Consequently, a significant amount of research has focused on identifying materials that possess a large magnitude of ZT. To obtain a large value of ZT, we employed nano-structuring and constructive modification of the electronic structure near the band edge using a small amount of a transition metal impurity element. The nanograined Si-Ge powder was prepared through high-energy planetary ball milling in an Ar atmosphere, and the resulting powder was sintered at a relatively low temperature under high pressure—873 K and 400-600 MPa. This process yields bulk samples of nano-grains with an average size of less than 10 nm, effectively reducing the lattice thermal conductivity to below 1 Wm⁻¹K⁻¹. We also added 1 at.% Fe as an impurity to create an impurity state nearthe bottom of the conduction band. As a result, the absolute value of the Seebeck coefficient was maintained ataround 400 μVK⁻¹ over a wide temperature range from 300 K to 1000 K. The large Seebeck coefficient of ~400µVK⁻¹, small lattice thermal conductivity lower than 1 Wm⁻¹K⁻¹, and relatively low electrical resistivity of a few mΩcm at high temperatures above 900 K resulted in a high ZT value of 1.88 at 900 K [1] and further increased to 3.6 at 1000 K [2]. Unfortunately, the samples prepared using the aforementioned process were often oxidized, resulting inhigher electrical resistivity. Despite maintaining a large Seebeck coefficient, the increased electrical resistivity naturally led to significant decreases in ZT. The inconsistent reproducibility of electrical resistivity has hindered ourability to prepare many high-ZT samples. Recently, we implemented a new method to eliminate oxidation during the sintering process. This methodproved effective, and the oxygen concentration was significantly reduced. Consequently, while maintaining a highSeebeck coefficient and low lattice thermal conductivity, the electrical resistivity was effectively decreased belowthat of the sample with the highest ZT value. Larger ZT values, specifically greater than 4, were thus achieved. This result suggests that our strategy worked well to effectively increase ZT of Si-Ge samples and presumably of other thermoelectric materials.

Energy-efficient synthesis of thermoelectric materials

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Abstract

The growing demand for sustainable energy solutions has accelerated the development of thermoelectric materials capable of directly converting heat into electricity. Traditional synthesis routes often require high temperatures and energy-intensive processes, limiting their scalability and environmental compatibility. In this study, we explore a series of energy-efficient synthesis techniques—such as hydrothermal, aqueous, and room-temperature methods—to fabricate both n-type and p-type thermoelectric materials, including Bi₂Te₃-, Cu₂Se-, PbSe-, Ag2Te-based composites, Cu_{1-x}Ni_x, Ni_{1-x}Cr_x alloys, and skutterudites. These methods not only minimize energy consumption but also enable precise control over microstructure, porosity, and carrier concentration, all of which critically influence the thermoelectric performance. Key materials synthesized via these low-energy approaches exhibit significantly enhanced power factors and figures of merit (zT), with some composites surpassing zT values of 1.0 at intermediate temperatures. The results affirm that energy-efficient fabrication routes are feasibler for achieving high-performance thermoelectric systems.

Hybrid Low-Dimensional TiO2 Photocatalysts: Role of Carbon and Metal Modification in Morphology and Pollutant Removal Performance
Rika Tri Yunarti, Universitas Indonesia, Indonesia

PFAS-Free Functional Polymers for High-Performance Triboelectric Nanogenerators and Sensors

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The development of high-performance triboelectric nanogenerators (TENGs) depends on polymer materials with optimized surface, electrical, and mechanical properties. Fluorinated polymers have been commonly used for their strong electron-withdrawing nature, but growing concerns over PFAS have created a need for safer alternatives.

In this work, we present a series of PFAS-free functional polymers—including plasticized PVC gels, engineering polyurethanes, and polyelectrolytes—designed for enhanced triboelectric and sensing performance. These materials were developed through controlled polymerization and molecular design, with tailored tribo-polarity and improved dielectric characteristics. Nanocomposite strategies further boosted charge storage via embedded dielectric and conductive fillers.

The resulting TENGs showed superior output performance and durability under mechanical stress. Additionally, the materials demonstrated high responsiveness to external stimuli, enabling reliable sensing for wearable electronics, soft robotics, and environmental monitoring.

Precise Synthesis of Advanced Conjugated Polymers for Efficient Perovskite Solar Cells Chang-Zhi Li, Zhejiang University, China

Cobalt Oxidation-State Engineering for Enhanced Electrocatalytic Water-Splitting in Copper-Cobalt-Based High-/Medium-Entropy Oxides

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Electrocatalytic water splitting involves the anodic oxygen evolution reaction (OER) and cathodic hydrogen evolution reaction (HER), with the sluggish four-electron OER being the rate-determining step. Replacing noble-metal-based catalysts with earth-abundant alternatives has driven extensive research into transition-metal oxides, particularly those containing cobalt. Variations in cobalt oxidation states critically affect catalytic activity; however, whether Co²⁺ or Co³⁺ predominates remains debated due to dynamic redox changes under electrochemical conditions.

In this work, we systematically investigate cobalt oxidation-state effects and compositional/structural influences on electrocatalytic performance using two complementary approaches. First, high-entropy and medium-entropy rock-salt oxides, (Mgo.₂Feo.₂Coo_{.2}Nio.₂Cuo_{.2})O and its four-cation derivatives, reveal that maximizing Co³⁺ concentration—achieved in the absence of Cu²⁺—yields the highest OER activity. Cu²⁺ is found to suppress the oxidation of Co²⁺/Fe²⁺ to Co³⁺/Fe³⁺, underscoring the importance of cation selection for oxidation-state tuning. Second, structurally distinct copper—cobalt oxides, delafossite-type CuCoO₂ and spinel-type CuCo₂O₄, are employed to stabilize cobalt oxidation states and enable controlled comparisons. CuCo₂O₄, with a higher Co³⁺/Co²⁺ ratio, exhibits superior bifunctional activity (OER: 317.9 mV; HER: 111.0 mV) compared to CuCoO₂ (OER: 404.4 mV; HER: 246.5 mV), alongside more favorable Tafel slopes.

These findings establish Co³⁺ as a key active species for OER in cobalt-based oxides, highlight the role of cationic composition and crystal structure in governing redox behavior, and provide design principles for high-performance, earth-abundant electrocatalysts based on high-/medium-entropy and spinel/delafossite oxides.

Development of Flexible Electrodes for Energy Storage and Sensing Applications Muhammad Iqbal, Institut Teknologi Bandung, Indonesia

Synergistic Dual-Site Janus MXene Quantum Dots for Sustainable Alcohol Oxidation

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The development of efficient, cost-effective, and environmentally benign catalytic systems is a critical priority for advancing green chemical processes. Selective oxidation of alcohols to aldehydes or ketones remains a fundamental transformation in fine chemical synthesis, yet conventional catalytic systems often rely on noble metals, which are costly, scarce, and environmentally burdensome.^{1,2} In this study, we report the design, synthesis, and catalytic evaluation of Janus Ni-MXene quantum dots (Ni-MJQDs) as a novel multifunctional catalyst for the selective oxidation of benzyl alcohol (BzOH) using peroxymonosulfate (PMS) as a green oxidant. This architecture combines the high surface-to-volume atomic ratio, tunable electronic structure, and asymmetrical surface functionalities of Janus materials with the redox-active nature of nickel, offering a unified strategy for enhancing catalytic efficiency.

The Ni-MJQD catalyst demonstrated outstanding performance in the selective oxidation of BzOH under mild aqueous conditions, achieving a conversion efficiency of 95% and a remarkable selectivity of 98.4% toward benzaldehyde. A high turnover frequency (TOF) of 8.8825 × 10⁻³ mol g⁻¹ h⁻¹ was recorded, which outperformed many existing non-

conditions, achieving a conversion efficiency of 95% and a remarkable selectivity of 98.4% toward benzaldehyde. A high turnover frequency (TOF) of 8.8825 × 10⁻³ mol g⁻¹ h⁻¹ was recorded, which outperformed many existing nonnoble metal catalysts. The catalyst exhibited excellent stability and reusability, retaining its catalytic activity over multiple cycles without significant structural degradation. Mechanistic investigations, supported by electron paramagnetic resonance (EPR) spectroscopy, scavenger studies, and Kinetic isotope studies (KIE), revealed that both radical and non-radical pathways were involved in the oxidation process. While PMS activation traditionally favors the generation of sulfate radicals, the unique electronic structure of the Ni-MJQD surface enabled electron transfer mechanisms that suppressed excessive radical formation and steered the oxidation reaction toward a more selective, non-radical route.

The Janus structure of the Ni-MJQD played a pivotal role in facilitating this dual mechanistic behavior. Asymmetric distribution of surface functionalities and Ni active sites promoted spatial charge separation and localized catalytic hotspots, thereby enhancing reaction kinetics while mitigating undesirable side reactions. The presence of abundant redox centers also contributed to efficient PMS activation and improved electron mobility across the interface, ensuring a consistent catalytic turnover. Furthermore, the hybridization of quantum-confined MXene domains with nickel atoms provided a robust and conductive framework. This work demonstrates that Janus Ni-MXene QDs are a promising, scalable catalyst for green alcohol oxidation, offering a sustainable alternative to noble metals through structural asymmetry, nanoscale effects, and surface redox synergy.

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Sunlight-Driven Photocatalytic Hydrogen Generation: Engineering Strategies for Sustainable Energy and Environmental Solutions Muthukonda Venkatakrishna Shankar, Konkuk University, South Korea

Thermal-to-Electrical Energy Conversion via a High-Efficiency, High-Power Air-Bridge III-V Thermophotovoltaic System

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With the growing demand for carbon neutrality, the development of highly efficient sustainable-energy systems has become increasingly vital [1]. Thermophotovoltaic (TPV) systems directly convert heat-driven infrared radiation into electrical power, decoupling energy generation from solar irradiance and enabling continuous operation across diverse thermal sources, such as concentrated solar heat, industrial waste-heat streams, and phase-change thermal storage. In this work, the principles of an air-bridge III-V TPV architecture capable of achieving high conversion efficiency and high power output are presented. Lattice-matched III-V free-standing thin films are suspended over an internal air cavity, maximizing photon recycling through highly reflective internal interfaces. Three critical design factors – emitter spectrum alignment, internal reflectivity, and membrane structural integrity – are systematically optimized via detailed fabrication protocols coupled with simulation-based design strategies. This air-bridge design not only improves optical performance but also enhances thermal and mechanical stability, enabling reliable, wafer-scale fabrication for practical deployment [2].

Under blackbody illumination at 1300-1400 K, the fabricated TPV cells achieve power conversion efficiencies exceeding 40% [3], where simulations indicate the potential to reach power densities greater than 5 W/cm² [4]. These results represent a significant advancement toward practical applications, such as concentrated solar power plants, industrial waste-heat recovery systems, and thermally powered remote sensors. Finally, strategies for realizing high-power-density TPV cells and integrating them with improved heat management are discussed, while maintaining high efficiency operation in next-generation clean-energy technologies.

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Synergistic Strategies for Low-PGM Electrocatalysts in HER and OER toward Efficient and Scalable PEM Water Electrolysis

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Engineering, Yonsei University, Seoul 03722, Republic of Korea E-mail address: hyunsoo.lim@keti.re.kr Electrochemical water splitting is a promising approach for high-purity hydrogen production without fossil fuel consumption or CO2emissions. Proton exchange membrane water electrolysis (PEMWE) offers distinct advantages, including low resistance losses, reduced gas crossover, and high current density. However, reliance on scarce platinum-group metals (PGMs), particularly Ir and Pt, remains a major barrier to commercialization. Therefore, rational catalyst design strategies that minimize noble-metal usage while maintaining high activity and durability are of critical importance. For the hydrogen evolution reaction (HER) at the cathode, two complementary approaches were explored. First, an inverted shell-core structure was developed in which Ir nanoparticles (1-2 nm) are encapsulated within a mesoporous carbon shell derived from polydopamine. This architecture achieved HER performance comparable to commercial Ir catalysts while reducing Ir content to below 1 wt%, demonstrating a shift from support-centered coatings to catalyst-centered support design. Second, mesoporous single-atom catalysts (MSACs) incorporating Ni centers were synthesized via metal chelation and soft-templating. Ni-MSACs exhibited superior stability, with overpotentials decreasing from 270 mV to 190 mV at 10 mA cm⁻² after 2,000 cycles, outperforming bulk Ni catalysts. Density functional theory calculations confirmed the Volmer-Heyrovsky pathway as the dominant HER mechanism, highlighting the critical role of isolated Ni active sites. Collectively, these results illustrate strategies for significantly reducing PGM content while maintaining high HER activity. In oxygen evolution reaction (OER) at the PEMWE anode, IrO2 remains the most reliable catalyst under harsh acidic and oxidative conditions. To overcome cost and scalability limitations, a modified Adams fusion method was developed, in which Ir precursors chelated with organic ligands were calcined in a LiNO3-KNO3 eutectic mixture instead of conventional NaNO3. The resulting IrO2 exhibited a distinct nanostructure and achieved overpotentials at 10 mA cm⁻² that were 25 mV lower than those from the standard Adams process and 45 mV lower than commercial IrO2. In PEMWE cells, the catalyst maintained excellent performance even at half the Ir loading of commercial benchmarks, demonstrating the feasibility of scalable and efficient Ir utilization. This study provides a systematic framework for the development of next-generation electrocatalysts. The inverted shell-core nanostructure and the single-atom HER catalysts for the cathode, together with the scalable synthesis of durable OER catalysts for the anode, work synergistically. Integrating these approaches enables substantial reductions in PGM dependence while achieving performance comparable to or exceeding that of commercial catalysts. Furthermore, this work addresses the economic and material limitations of PEMWE, offering a pathway toward large-scale, costeffective hydrogen production that contributes to the transition to clean energy.

Single-Atom Decorated Platinum for High-Performance Ammonia Oxidation

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The global warming crisis, largely driven by increasing CO_2 emissions, necessitates innovative solutions to mitigate its impact. One of the promising strategies is the utilization of ammonia as a hydrogen carrier. Ammonia, a carbon-free substance with a higher energy density than hydrogen gas, offers significant advantages in terms of handling and transportation. However, a major challenge in utilizing ammonia in fuel cells is the instability of the anodic ammonia oxidation reaction (AOR). The catalysts required for the AOR is susceptible to poisoning from nitrogen-based intermediates, such as adsorbed nitrogen (N_{ads}) and nitric oxides (NO_{Xads}). These poisoning effects hamper the efficiency and lifetime of the catalysts. Recent research has explored the introduction of transition metals into the catalyst matrix as a potential solution to these issues. Transition metals such as N_1 and N_2 have shown promise in enhancing the stability of the catalysts by mitigating the poisoning effects. Although their beneficial impacts have been well documented, the exact mechanisms by which they improve resistance to poisoning are not fully understood. In this presentation, we examined the effects of incorporating various transition metals at the atomic level onto the surface of platinum nanocubes. By testing these modified catalysts, we aim to better understand their effectiveness in facilitating the AOR and improving overall performance. This approach could provide significant advances in the development of more efficient and durable ammonia-based energy systems.

Ion Conducting Membranes through Self-Assembly of Graft Copolymers
Jong Hak Kim, Yonsei University, South Korea

Aluminosilicate-Reinforced Graphene Oxide Membranes with Tunable Hierarchical Spacings for Electrochemical Lithium Recovery Beyond the Selectivity-Permeability Trade-off

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Strategies for High-Performance Aqueous Rechargeable Zinc Batteries

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Aqueous Rechargeable Zinc Batteries (ARZBs) have been greatly increasing in interest for application to large scale energy storages (ESSs) owing to their advantages in terms of high power, low cost, and safety. Despite such high interest, there are still limitations in improving the performance of ARZBs due to the absence of high-performance cathode materials and the dendrite growth of Zn anodes. To solve this problem, we paid attention to supramolecular chemistry for developing a high-performance cathode and controlling an anode-electrolyte interfaces. In particular, for the cathode material, high capacity and high output characteristics were realized through the development of a redox-active triangular phenanthrenequinone-based macrocycle (PQ- Δ) and Cu₃(HHTP)₂, a conductive 2D MOF cathodes with a hydration effect. Furthermore, UiO66-(Zr)-(COOH)₂ and supramolecular MOF were introduced as artificial interfacial layers to effectively control dendrite growth on the Zn anode during battery operation. Therefore, it was possible to present key insights for high performance ARZBs.

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Material design of conductive oxide semiconductor films to achieve thickness-dependent properties for a wide range of applications

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We have developed highly transparent conductive oxide (TCO) films based on n-type doped ZnO and In2O3 films with thicknesses (t) ranging from a few nanometers to micrometers [1]. Our main concern is how to achieve high carrier transport, such as 145 cm2 /(Vs) [2] and so on, at high carrier concentrations (N) ranging from 2×1020 to 2×1021 cm-3, independent of the thickness. The N values are strongly dependent on the applications, including transparent conductive electrodes with t ranging from 100 to 150 nm for solar cells [2], liquid crystal displays (LCDs) [3,4] and short-wavelength light-emitting diodes, and electromagnetic shielding with t of more than 1 micrometers, gas sensors with t of 50nm [5], γ radiation resistance with t of 200 nm [6] required for the foreseeable future in space, and antibacterial with t of 50nm for human healthcare. Our TCO thin films have been implemented in some applications and are commercially available[1]. The developed deposition technology, called reactive plasma deposition with direct current arc discharge, which is commercially available trough the collaboration with Sumitomo Heavy Industries, Ltd, [1] enables with fast film growth, such as typically 200 nm/min, large scale deposition on substrates with a size of 1×1 m2 square, and low deposition temperature in the range of room temperature to 250 °C. This allows the use of polymer-based substrates as well as that of glass substrates. We have found a thickness-dependent elastic modulus for Ga-doped ZnO (GZO) polycrystalline films consisting of a welldefined (0001) preferentially oriented columnar structure [7.8]. We have, thus, achieved flexible polymer substrates deposited with GZO-based TCO films with t of 30nm. The composite films show bending-resistant feature in electrical properties. Very recently, we have realized high Hall mobility W-doped In2O3 with thicknesses below 10 nm [9]. In this talk, we discuss how to achieve TCO films with high carrier transport and, moreover, elucidate the physics characterizing the free electron system.

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Molecularly Engineered Nanoplatforms for Selective Detection and Neutralization of
Molecular Threats
Young Hun Seo, KIST Europe, Germany

Stimuli-Responsive, Morphology-Switching Bottlebrush Copolymer Particles Shin Jaeman, Soongsil University, South Korea

A Shock Tube Investigation of Structural, Morphological and Photocatalytic Properties of Strontium Stannate Nanostructures

Sivaprakash Paramasivam, Keimyung University, South Korea

Resolving Intrinsic 3D Structural Variations in Nanoparticles *via* Liquid-Phase Electron Microscopy

Byung Hyo Kim, Soongsil University, South Korea

Development of LiDAR-Detectable Black Materials *via* Various Strategies and Their Application as Eco-friendly Paints for Autonomous Driving Environments Chang-Min Yoon, Inha University, South Korea

Insights of Carbon-Material Stabilized Nano-Metallic Catalysis to Boost C–C Bond Formation/polymerization Md. Shahajahan Kutubi, Nagoya University, Japan

Synthesis-with-direction of Gold Nanoparticles by DNA Ma Xingyi, Harbin Institute of Technology, China

Three-Dimensionally Nanofabricated Ir Nanoarchitecture Electrode for Highly Efficient and Robust PEMWE

Jong Min Kim, Korea Institute of Science and Technology (KIST), South Korea

TBA

Jing Tang, East China Normal University, China

Designing multifunctional waterborne polymer nanocomposites

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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 wellestablished 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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Boosted Performance and Stability in LaFeO_/MXene/rGO Nanocomposites through Dual-Conductive Network for Supercapacitor Energy Storage Application Harish Verma, Indian Institute of Technology (B.H.U.) Varanasi, India

Safe-by-Design Nano-Enabled Food Packaging: Mechanistic Insights and Material Strategies to Mitigate Nanoparticle Migration

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Abstract

Integrating nanoscale fillers such as zinc oxide (ZnO), silver (Ag), nanoclays, and titanium dioxide (TiO₂) into polymer matrices has transformed food packaging. These nanocomposites provide superior barrier properties, UV protection, and antibacterial-aid, addressing the global need for extended food shelf life and reduced spoilage. However, uncontrolled nanoparticle migration from packaging into food, particularly under increased temperature, acidity-based systems, or high-fat systems has raised major toxicological, regulatory, and consumer acceptance concerns [1].

This work presents a **materials engineering perspective** to study migration mechanisms as well as structure-property relationships and design strategies for safe and high-performance nano-enabled packaging. A critical survey of recent literature depicts how nanoparticle characteristics (size, morphology, surface chemistry) mixed with polymer-filler interactions regulate migration kinetics. Migration is typically studied in vitro by exposing packaging materials to food simulants under controlled lab conditions. Traditional diffusion models, such as Fick's laws, generally fail to predict the nanoparticle behaviour because these laws assume small, non-interacting molecules. In contrast, nanoparticles exhibit complex interactions, including matrix bonding, agglomeration, and reabsorption, reducing predictability. Comparative data analysis highlights material-specific behaviour: for instance the migration of AgNP sometimes exceeded 12.9 mg/kg in acidic simulants, [2] and over 30.85 mg/kg of ZnO release was observed from PBAT/TPS films stored at 40 °C [3], violating EFSA's limit of 0.05 mg/kg for silver [4] and 5 mg/kg for Zn [5] in food-contact materials. These findings underscore the need for improved models and design approaches. Drawing from these considerations, a safe-by-design framework is proposed, specifying methods such as nanoparticle encapsulation by inert coatings, multilayer barrier structures, covalent surface functionalisation, and hybrid filler systems that block mobility while maintaining performance. Key parameters include: scalability; long-term stability; and compatibility with current processes.

The study also identifies **regulatory gaps** across global jurisdictions, including inconsistent migration limits, lack of nanoparticle-specific assessment models, and absence of harmonised testing protocols. Recommendations include developing predictive modelling accounting for particle–polymer binding dynamics and storage conditions, along with a relatively transparent labelling policy to foster consumer trust. By mixing materials science with toxicology and policy considerations, this work sets a technical groundwork and strategic pathway for sustainable, safe, and high-performance food packaging system.

Current Rectification in a Sub-2nm Vertical PN Diode

Van Dam Do, Sungkyunkwan University, South Korea

Poly(2-ethyl-2-oxazoline)-Conjugated Hemoglobins: Artificial O2 Carriers as Red Blood Cell Substitutes

Teruyuki Komatsu, Chuo University, Japan

Intermolecular FRET can be Utilized for Evaluations of Lectin—Carbohydrate Interactions

Koji Matsuoka, Saitama University, Japan

A Multifunctional, Transparent, Adhesive, and Antioxidative Hydrogel for Minimally Invasive Therapy for Retinal Tissue Repair

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Oxidative stress, primarily triggered by an increase in reactive oxygen species (ROS), is a significant factor in the pathology of various retinal diseases. To counteract this, we developed GelCA-2OH and GelCAo-2OH, advanced hydrogels engineered with caffeic acid chemically conjugated to the gelatin backbone and stabilized through microbial transglutaminase for in situ crosslinking. These hydrogels, leveraging the antioxidative properties of caffeic acid, demonstrated enhanced injectability, self-healing capabilities, and excellent biocompatibility and biodegradability, making them ideal for retinal applications. In retinal injuries models, they significantly reduced ROS levels and promoted cellular recovery, highlighting their transformative potential in regenerative medicine and biomedical engineering. This research underscores the promise of caffeic acid-modified gelatin hydrogels as a novel therapeutic tool for oxidative stress in ocular tissues, opening new avenues for clinical research and offering promising strategies for restoring vision in retinal diseases traditionally considered difficult to manage.

Micropatterned Bioresponsive Hydrogel for Real-Time and Label-Free Monitoring
Proteins and Cell Behaviors
Won-Gun Koh, Yonsei University, South Korea

Multifunctional Nanoparticles: Design, Antibacterial Applications, and Mechanistic Studies (Online) Jun Wang, Anhui Polytechnic University, China

WR-3.4 Hollow-Waveguide Mach-Zehnder Interferometer Composed of Two Y-Branch Structures Fabricated Using a 3D Printer and Metal Plating

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This work demonstrates a waveguide-based Mach–Zehnder interferometer (WG-MZI) operating in the terahertz (THz) band, fabricated using our in-house UV-curable 3D printer (RECILS) combined with electroless metal plating.[1] The goal is to realize compact, stable, and portable interferometers suitable for THz applications such as gas sensing and refractive index measurements. Conventional free-space interferometers in the THz band suffer from alignment challenges and limited component availability. While waveguide optics is a promising candidate to overcome these issues, fabricating THz-band waveguides is difficult because sub-millimeter hollow structures must be formed within metal blocks.

RECILS enables monolithic fabrication of sub-millimeter-scale hollow structures with arbitrary freeform geometries. By plating the inner surfaces with Ni and Cu, functional hollow waveguides for the THz band can be realized. This method allows the construction of intricate structures—such as bandpass filters, Y-branch splitters, and spiral waveguides—that are challenging to fabricate with traditional split-block approaches.

The WG-MZI is formed by combining two Y-branch waveguides, each enclosed within a one-inch-long body and equipped with UG-387 flanges for straightforward connection. The two branch waveguides of one Y-branch couple to those of the second Y-branch via the flanges. At the branch point of the first Y-blanch waveguide, a mode converter transforms the input TE10 mode into a TE20 mode, reducing the electric field at the split and minimizing loss. The divided TE10-mode signals then propagate separately and recombine at the second Y-branch, producing interference characterized by the arm length difference (ΔL).

We fabricated and tested WG-MZIs with different ΔL values. For $\Delta L = 12$ mm, transmission measurements near 300 GHz showed interference fringes with a free spectral range (FSR) of ~20 GHz, an insertion loss of ~4 dB, and an extinction ratio greater than 15 dB. When ΔL was reduced to 0 mm, the fringes disappeared, confirming proper interferometer operation. A device with $\Delta L = 18.4$ mm exhibited fringes with an FSR of ~10 GHz, consistent with theoretical predictions. Spiral 3D waveguide structures were employed to realize longer path differences within compact footprints, demonstrating the advantages of freeform 3D fabrication.

In conclusion, this study demonstrates that combining our in-house 3D printing technology, RECILS, with electroless plating enables compact, low-loss, hollow waveguide THz interferometers. The fabricated devices exhibited clear interference with high extinction ratios, verifying their functionality. Future work will focus on improving performance and integrating semiconductor chips into one interferometer arm, enabling applications such as modulators and sensors.

This approach establishes a promising pathway toward practical, portable, and cost-effective interferometric devices for THz sensing and communication.

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Advances and Emerging Trends in Medical Applications of Diamond-Like Carbon (DLC) Coatings

Yasuhiro Fujii, Okayama University, Japan

Multiplexed Ultrafast Photothermal Digital PCR based on Oligo(Phenylene-Ethynylen) Interfacing Compound

Oh Seok Kwon, Sungkyunkwan University, South Korea

Peptide-Based Biomimetic Nanoparticle Vaccines against Breast Cancer: Prophylactic and Therapeutic Modalities

Fazren Azmi, National University of Malaysia, Malaysia

Biomimetic Nanotechnology-Mediated Physical Bioregulation to Induce *In-situ* Tissue Regeneration

Masahiro Yamada, Tohoku University Graduate School of Biomedical Engineering, Japan

Self-Assembly of Amorphous and Functional Polymer Nanodiscs in Water

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Polymer nanodiscs are challenging to make.^[1] This is because self-assembly processes typically yield micelle shapes of minimised energy, like spheres or vesicles. Flattening such assemblies is more intricate, as block ratios and solvent—polymer interactions alone cannot compensate for the energy costs to flatten a curved surface or interface. Taking on this challenge, we designed an amphiphilic, tadpole-like copolymer featuring a hydrophilic linear block and a hydrophobic bottlebrush block. The linear segment assumes a coil-like conformation, while the bottlebrush segment adopts a stiffened, rod-like structure. Using this rod-coil architecture facilitated planar packing of brush segments and yielded nanoscale polymer discs via spontaneous self-assembly. A characteristic feature of this methodology is the possibility to select the chemical composition of the brush segment without compromising the disc formation. This allows the introduction of functionality into these amorphous core-shell nanodiscs, enabling triggered disassembly and/or drug release, depolymerisation, or shape-transformation.^[2, 3] My talk will introduce our general approach.

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Soft Sensing Fibers with Chemically Embedded Nanoparticles for Biomedical and Biomechanical Applications

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Immune-modulative nano-gel-nano for patient-favorable cancer therapy

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Current cancer immunotherapies exhibit low response rates attributed to suppressive tumor immune microenvironments (TIMEs). To address these unfavorable TIMEs, supplementation with tumor-associated antigens and stimulation of immune cells at target sites are indispensable for eliciting anti-tumoral immune responses. Previous research has explored the induction of immunotherapy through multiple injections and implants; however, these approaches lack consideration for patient convenience and the implementation of finely tunable immune response control systems to mitigate the side effects of over-inflammatory responses, such as cytokine storms. In this context, we describe a patient-centric nano-gel-nano system capable of sustained generation of tumorassociated antigens and release of adjuvants. This is achieved through the specific delivery of drugs to cancer cells and antigens/adjuvants to immune cells over the long term, maintaining proper concentrations within the tumor site with a single injection. This system demonstrates local immunity against tumors with a single in jection, enhances the therapeutic efficacy of immune checkpoint blockades, and induces systemic and memory T cell responses, thus minimizing systemic side effects.

Van der Waals 3D Assembly of 2D Nanomaterials for Scalable Electronics <u>Joohoon Kang</u>, a*

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Two-dimensional (2D) nanomaterials have received great attention as potential building blocks for use in fundamental elements of (opto)electronic applications due to their diverse and remarkable electronic and optical properties. However, such fundamental demonstrations cannot be directly applied to practical applications because of scalable synthesis of high-quality nanomaterials and their proper assembly. In this presentation, I will demonstrate wafer-scale van der Waals assembly of 2D materials, which are exfoliated via a molecular intercalation-assisted electrochemical exfoliation method. The resulting materials with distinct electronic properties including metal, semiconductor, and insulator, can be assembled into various (opto)electronic devices such as transistors, diodes, logic gates, and photodetectors. Also, such solution-based approach further enables inkjet printing-based device fabrications without conventional lithography.

Development of Lensless Light-Sheet Sources and their Application for 3D Imagingin Bio and Medical Science (Online)

Junji Yumoto, Soongsil University, South Korea

Surface-enhanced Raman Scattering Properties of Gold-open Shell Nanoprobes and their Application to Cell Imaging Yuka Hori, Nihon University, Japan

International Conference on Materials Science and Engineering (Materials Oceania 2025) September 16-19, 2025 | Yonsei University, Seoul, South Korea

Flexible Smart Knee Sleeve Integrating Textile Pressure Sensors and IMUs for LowerLimb Rehabilitation Monitoring

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Abstract: Monitoring lower-limb rehabilitation requires accurate assessment of both joint kinematics and muscle activity to guide recovery from diverse injuries such as ligament tears, meniscal damage, and post-surgical interventions. Wearable biomaterials offer a promising pathway to transform rehabilitation monitoring by enabling continuous, portable assessment of musculoskeletal function. In contrast, conventional laboratory-based methods such as motion capture and electromyography (EMG) deliver reliable results but remain costly, immobile, and impractical for daily use.

To address this gap, we developed a flexible smart knee sleeve that integrates fourteen textile-based pressure sensors positioned across the quadriceps, hamstrings, calf, and shin, together with dual nine-axis inertial measurement units (IMUs). This bio-integrated sleeve captures multimodal time-series signals of muscle activation surrogates and joint motion, streaming them wirelessly through a lightweight custom interface. Clinical and technical validation demonstrates its ability to provide actionable feedback: range of motion estimates benchmarked against motion capture achieve a mean absolute error of 7.21° (within clinical thresholds), while muscle activation patterns derived from textile pressure sensors correlate strongly with EMG references (normalized RMSE = 0.27).

Building on this sensing foundation, we introduce a multi-task deep learning framework (BFMT-Net) that jointly performs injury state recognition and exercise classification. By leveraging conditional sensor attention to fuse pressure and inertial features, the framework reduces false negatives and false positives, thereby improving decision-making reliability for personalized rehabilitation.

Evaluation across both patients and healthy adults confirms consistently high recognition accuracy, with intersubject performance above 90% and intra-subject performance exceeding 96% for injury and exercise detection. Among healthy participants, exercise recognition surpasses 96% inter-subject and 98% intra-subject accuracy, underscoring broad generalizability. Furthermore, the system operates in real time at 0.281 GFLOPs with <50 ms inference latency, enabling seamless feedback on both range of motionand muscle activation during rehabilitation tasks.

By combining textile-based biomaterials with multimodal sensing and efficient machine learning, the smart knee sleeve establishes a clinically validated pathway for personalized rehabilitation monitoring. This integration of pressure and inertial data into a real-time bioengineering platform demonstrates how wearable systems can extend precision monitoring beyond the laboratory, ultimately empowering clinicians and patients to optimize recovery outcomes.

Keywords: smart biomaterials, textile-based pressure sensors, wearable bioelectronics, lower-limb rehabilitation,

multimodal sensing, personalized rehabilitation monitoring

Anisotropic Spin Hamiltonian Generalized for NiPS3
Myung Joon Han, Korea Advanced Institute of Science and Technology (KAIST), South Korea

Synthesis of Van der Waals Heterostructure via Chemical Vapor Deposition Ki Kang Kim, Sungkyunkwan University, South Korea

International Conference on Materials Science and Engineering (Materials Oceania 2025) September 16-19, 2025 | Yonsei University, Seoul, South Korea

Development of Red and Infrared Emitting Scintillators with High Emission Efficiencies

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Real-time dose monitors are required under high-dose-rate conditions to remove debris at the Fukushima Daiichi Nuclear Power Plant as part of the decommissioning step. Scintillator is one of the optical materials used to detect radiation, and conventional scintillation materials have emission wavelengths of 300-550 nm. However, the above application, novel material with longer emission wavelengths and relatively high mission intensity are required to have higher sensitivity under such high dose rate. I have developed a dose monitor for this application using scintillation material with a long emission wavelength (550-1000 nm) and high light output. For example, Cs2Hfl6 and Rb2Hfl6 were used for gamma-ray detection, and Li2HfBr6 was sensitive to both gamma rays and neutrons. These scintillators had light outputs of 20,000 – 70,000 photons/MeV, which can be classified as the high light-output group compared to conventional materials with blue emission, and these emission wavelengths were 600 to 750 nm. In this paper, I show the above results, including the development of the monitor and other optical properties such as temperature dependence for the light output, and discuss the relationship between the crystal structures and optical properties.

Influence of Plasmonic Metal Nanostructures on Triplet-Triplet Annihilation Upconversion Kosuke Sugawa, Nihon University, Japan

Acoustic Shock Wave-Induced Phase Transitions in Solid-State Materials via Dynamic Recrystallization: Case Studies and Insights
S.A. Martin Britto Dhas, Keimyung University, South Korea

Artificial Synaptic Devices for Physical Reservoir Computing Hongseok Oh, Soongsil University, South Korea

High-Purity Low-Radioactive Background Materials for Extremely Rare-Event Physics at CUP

Olga Gileva, Institute for Basic Science (IBS), South Korea

High Performance of Ti-Ge-Te Thin Film for Flexible Electronics Application

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Abstract: The flexible titanium-doped GeTe phase change material was proposed and fabricated by magnetron cosputtering method. The impact of titanium dopant and mechanical bending on the thermal stability, electrical resistance, surface morphology, microstructure and crystallization mechanism of GeTe thin film were investigated systematically. With the incorporation of appropriate titanium dopant, the crystallization process can be hindered and grain size can be limited, respectively. Meanwhile, the thermal stability, surface morphology and crystal structure have not been changed obviously when the bending times reaching 10⁶, demonstrating the distinguished bending performance. The density functional theory calculations of band structure illustrate that titanium dopant can convert the indirect band gap to the direct one of GeTe material. The formation energy and charge density difference indicate the massive electron cloud agglomerate between the Ti and Te atoms, deducing that the foreign Ti may occupy the position of Ge and form the covalent bonds with Te. Both the experimental and theoretical analysis prove that the nanoscale Ti-Ge-Te thin film possess the outstanding crystallization behavior and flexural performance, which has the immense potential for the flexible memory application.

Demonstration of Time-Reversal Symmetry Breaking in Chiral Terahertz Photonic-Crystal Cavities

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Light-matter interactions in chiral cavities offer a promising approach to control material properties by breaking fundamental symmetries like time-reversal or inversion symmetry. To date, only a few demonstrations of chiral cavities exhibiting time-reversal symmetry breaking have been reported. These implementations typically require the application of a strong magnetic field or the hybridization of cavity modes with matter excitations in the ultrastrong coupling regime. Here, we present a one-dimensional terahertz photonic-crystal cavity in which time-reversal symmetry is broken [1]. Our cavity consists of an undoped silicon layer sandwiched between lightly n-doped InSb wafers. By leveraging the nonreciprocal properties of a terahertz magnetoplasma and the low effective mass of electrons in InSb, we confined a cavity mode with a single circular polarization at 0.67 THz in the presence of a small (~0.3 T) magnetic field, achieving a Q-factor exceeding 50. Temperature, magnetic field, and polarization-dependent experiments and simulations validate the proof-of-concept chiral cavity with broken time-reversal symmetry, making it well-suited for studies of chiral light-matter interactions in the terahertz range.

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Strategic Electrolyte Design for Highly Nonvolatile Artificial Synapse Eunho Lee, Seoul National University of Science and Technology, South Korea

Extended-Gate-Type Organic Field-Effect Transistors for Chemical Sensing Applications
Tsuyoshi Minami, The University of Tokyo, Japan

Performance of Lead-Free Cs2TiI6-MoS2-based Solar Cell Structure Arpana Agrawal, Shri Neelkantheshwar Government Post-Graduate College, India

Energy Harvesting via Hydrophobic Hydration Membrane Yong Whan Choi, Silla University, South Korea

International Conference on Materials Science and Engineering (Materials Oceania 2025) September 16-19, 2025 | Yonsei University, Seoul, South Korea

Boosting Oxygen Reduction Reaction with Single-Atom Fe Anchored on Hollow N-Doped Carbon

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Abstract: Over the past several decades, fuel cell systems have emerged as a high-priority research area, driven by the need to enhance performance in response to growing energy demands. The oxygen reduction reaction (ORR) plays a crucial role in fuel cell systems, requiring a catalyst due to their inherently slow kinetics. Various catalysts studied, transition metal-decorated nitrogen-doped carbon materials have demonstrated limited success in achieving the desired levels of activity, durability, and cost-effectiveness. Consequently, the rational design of porous nanostructured carbon-based catalysts with abundant active sites is essential for improving catalytic performance. Numerous ORR catalysts have been investigated using different metal and carbon material combinations to enhance efficiency and stability. Å In the present study, we developed a novel electrocatalyst for the ORR achieved through a simple pyrolysis process of hemoglobin-adsorbed phenolic resin nanoparticles, followed by acid etching. The FehNC exhibits a uniform spherical shape with an average diameter of approximately 500 nm. XRD analysis revealed characteristic peaks corresponding to carbon, with no discernible diffraction peaks for crystalline Fe-based species, likely due to the low iron content. Peaks associated with structural defects and graphitic features were also observed. Nitrogen adsorption—desorption isotherms of FehNC indicated a high specific surface area of 822.5 m²/g, and pore size distribution analysis confirmed the presence of micropores (<2nm). ICP-OES analysis quantified the iron content at a trace level of 1.31%. High-resolution XPS spectra of the N 1s region displayed four deconvoluted peaks attributed to graphitic, pyrrolic, and pyridinic nitrogen species. Among these, pyridinic and graphitic nitrogen are known to enhance catalytic activity by providing additional active sites for the oxygen reduction reaction (ORR). The nitrogen binding configuration within the carbon matrix was further elucidated using N K-edge X-ray absorption near-edge structure (XANES) spectroscopy. Fe K-edge XANES and Fourier-transformed extended X-ray absorption fine structure (EXAFS) spectra were analyzed to determine the oxidation state of iron and the local coordination environment in the Fe-N-C active sites. The EXAFS spectrum of FehNC exhibited a prominent peak at approximately 1.64 Å, corresponding to the Fe-N scattering path. Notably, the absence of a Fe-Fe scattering peak near 2.1 Å confirmed the atomic dispersion of iron, indicative of single-atom catalyst characteristics. Electrochemical measurements demonstrated that the FehNC catalyst exhibits superior ORR activity compared to nitrogen-doped carbon, with an onset potential of 0.916 V vs. RHE and a half-wave potential of 0.833 V vs. RHE in alkaline media. The catalyst retained 80–90% of its initial current density after 15 hours of durability testing, indicating excellent operational stability. Theoretical calculations further confirmed that the enhanced catalytic activity of FehNC, particularly under alkaline conditions, can be attributed to the functionalization of Fe sites by hydroxyl groups. This facilitates *OH desorption by bypassing the clean surface state, effectively improving the ORR kinetics. These results emphasize the importance of regulating both the local coordination structure of active sites and the particle-level morphology for optimizing electrocatalytic performance. In conclusion, we successfully synthesized a high-performance, trace Fe-anchored carbon catalyst (FehNC) with a hollow structure suitable for ORR. The nitrogen-doped hollow carbon matrix enhances mass transport and electron transfer during ORR, while the uniform distribution of trace Fe atoms introduces additional catalytic sites, contributing to superior ORR activity. This innovative approach, which integrates hollow carbon morphology with Fe precursor engineering and theoretical insights into site reactivity, provides a promising strategy for designing advanced electrocatalysts for energy conversion applications.

Racolyte: A Raman Spectra Identification Software of Mineral Materials Huei-Fen Chen, Institute of Earth Sciences, National Taiwan Ocean University, Taiwan

Current Rectification in a Sub-2 nm Vertical PN Diode

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Vertically stacked PN heterojunctions (VPNJ) have shown significant promises for a wide spectrum of electronic and optoelectronic applications, due to the robust light-matter interaction, typical optical and atomic thin structures. Monolayers vertical PN heterojunctions with planar-contacted electrodes (1Ls-VPNJ-PE) exhibit current rectification, but it originates from bending in the non-overlapped region along the lateral direction. 1Ls-VPNJ with vertically stacked graphene electrodes (1Ls-VPNJ-VE) has been reported for a PN photodiode to minimize interlayer recombination losses^[1]. However, the high tunneling current across the large overlapping junction area overshadows the relatively small rectification current of the PN diode.

Here, we demonstrate for the first time current rectification in a sub-2 nm channel-length 1Ls-VPNJ-VE structure consists of a vertically stacked carbon nanotube (CNT)/ monolayer V-doped WS₂ (p-type)/ monolayer MoS₂ (n-type)/ CNT (C/V.W/M/C). Our C/V.W/M/C structure features an ultra-narrow contact area, which suppresses the tunneling current to below 10 pA, thereby allowing the rectification current to dominate the total current flow. We propose a new model for the 1Ls-VPNJ-VE, in which the van der Waals (vdW) gap between the p-type and n-type monolayers prevents electrostatic coupling, enabling independent potential modulation in each monolayer. As a result, the built-in potential changes dynamically under forward and reverse bias, leading to clear rectification behavior. Additionally, the 1Ls-VPNJ-VE exhibits negative photoconductivity, attributed to an increased Schottky barrier at the CNT_B/V.WS₂ interface due to the trapping of photogenerated electrons in V-induced trap states. Benefiting from fast charge transfer in vertical vdW heterostructures, our 1Ls-VPNJ-VE demonstrates fast photoresponse with fall and rise times of 0.9 μ s and 1.1 μ s, respectively-approximately 100 times faster than the previous 1Ls-VPNJ-PE.

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Toward Accurate Crack Detection in Ceramics: Semantic Segmentation with Limited Training Data

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Synthesis of Polymer-Based Tubular Micromotors Capable of High-Density Drug Delivery and Light-Triggered Release

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Swimming tubular micromotors with autonomous propulsion in physiological environments have attracted much attention for active drug delivery systems. ¹⁾ If self-propelled micromotors deliver therapeutics to the target site and external stimuli facilitate local release, highly efficient therapy with minimal side effects would be possible. The aim of this study is to synthesized polymer-based tubular micromotors with urease (Ure) immobilized on the inner surface and doxorubicin-loaded liposomes (DoxL) attached to the outer surface (DoxL/Ure tube micromotors), and to investigate their self-propulsion capabilities, drug release by near-infrared (NIR) irradiation, and anticancer efficacy.

The desired tubular micromotor was synthesized through a four-step process. In the first step, bis{2-(methacryloyloxy)ethyl} phosphate (BMP) was photopolymerized into a porous polycarbonate (PC) membrane (pore diameter: 8.0 μm; thickness: 18 μm) by UV irradiation. In the second step, avidin (Avi) were deposited in the pore by layer-by-layer assembly. Dissolution of the PC template provided uniform hollow cylinders (Avi tubes). In the third step, biotinylated Ure (bUre) was immobilized as the innermost layer using avidin-biotin interaction. The obtained Avi tubes were soaked into aqueous bUre solution, resulting in the Ure tubes. Finally, DoxL was electrostatically adsorbed onto the outer surface of the Ure tube. DoxL was prepared using a remote loading procedure. After inserting the fluorescent molecule DiD between the bilayers of liposomes composed mainly of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine and 1,2-dipalmitoyl-sn-glycero-3-ethyl-phosphocholine (a cationic lipid), doxorubicin was encapsulated in the internal aqueous phase. DoxL was added to the PBS dispersion of Ure tubes to yield DoxL/Ure tubes (outer diameter: ca. 8.0 μm, tube length: ca. 18 μm).

The obtained DoxL/Ure tubes exhibited a pronounced roughness on the outer surface, indicating DoxL adsorption. Furthermore, DoxL/Ure tube micromotors swam in aqueous urea solution while retaining surface-adsorbed liposomes (11.4 μ m/s). The propulsion mechanism attributed to self-diffusion of CO₂ and NH₃ produced by urea decomposition. To achieve externally triggered drug release, NIR light was used to locally heat the DoxL/Ure tube dispersion. Upon NIR irradiation, localized heating raised the temperature above the gel-to-liquid crystalline phase transition temperature (T_c : 38.5 °C) of the liposomes, inducing rapid Dox release. After 5 min of irradiation, 76.4% of the encapsulated Dox was released.

The cytotoxicity of DoxL/Ure tube micromotor was evaluated using breast cancer cells, MCF-7. When introduced into a cell culture supplemented with urea, the self-propulsive motion of the micromotors facilitated enhanced cell interaction. Subsequent NIR irradiation triggered localized Dox release in the vicinity of the cancer cells, and cell viability was reduced to $19 \pm 4\%$ compared to the control value, indicating efficient cell death. The DoxL/Ure tube micromotors, capable of high-density drug delivery and on-demand light-mediated release, represent a promising biotool for active drug delivery.

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Polymerized Stromal-Free Hemoglobin Nanoparticles Coated with Serum Albumin as a Red Blood Cell Substitute

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In contemporary medicine, blood transfusion is a critical procedure that saves countless lives. However, reliance on donations from healthy individuals raises concerns about future blood shortages, particularly with declining birth rates and aging population. Under such background, achievement of red blood cell (RBC) substitutes is widely required. Over the past several decades, various hemoglobin (Hb)-based O₂ carriers (HBOCs) have been developed. Nevertheless, there are two critical challenges. First, adverse effects such as vasoconstriction and hypertension caused by the leakage of HBOCs from blood vessels. Second, the oxidation of ferrous-heme iron, which binds O₂, cannot be prevented. In contrast, stromal-free Hb (SFHb) removed cell membrane from RBC contains antioxidant enzymes (catalase (Cat) etc.), which protects heme against autooxidation.

In this study, we described core-shell structured nanoparticle comprising a polymerized SFHb core and human serum albumin (HSA) shell, SFHbNP.¹⁾ After the introduction of maleimide groups to Lys residues of SFHb using *N*-succinimidyl 3-maleimidopropionate, the obtained SFHb was crosslinked using dithiothreitol, yielding SFHb microsphere. Subsequently, the remaining maleimide groups on the particle were conjugated with the Cys-34 residue of HSA, resulting in core-shell structured SFHbNP. With an optimized particle size of approximately 30 nm, SFHbNP is engineered to evade uptake by the reticuloendothelial system in various organs. The SFHbNP dispersion did not occur precipitation and aggregation over one year, demonstrating superior stability. SFHbNP exhibited a moderately high O₂ affinity (P₅₀=8 Torr) facilitating efficient O₂ transport to hypoxic tissues, particularly in hemorrhagic shock scenarios. SFHbNP^L prepared using deoxy (T-state) Hb in an N₂ atmosphere showed low O₂ affinity (P₅₀=59 Torr). It is remarkable that the mixing of SFHbNP and SFHbNP^L in proper ratios conferred a tailor made formulation with a desired P₅₀ value (9-59 Torr). Moreover, the antioxidant ability of SFHbNP was evaluated under physiological conditions. The SFHbNP in PBS solution containing 20 μM H₂O₂ (mimic plasma concentration) did not exhibit heme oxidation. This effect is attributed to trace amounts of Cat, which decomposes H₂O₂ into H₂O and O₂, a potent antioxidant enzyme encapsulated within the core of SFHbNP.

The resuscitation efficacy of SFHbNP was investigated using a rat model with 50% blood volume exchanged, stimulating severe hemorrhagic shock. All rats treated with SFHbNP survived following resuscitation. The mean arterial pressure and heart rate decreased by hemorrhagic shock and quickly returned after SFHbNP injection. The results exhibited excellent resuscitative efficacy. Given its antioxidant properties and long-term storability, SFHbNP emerges as an excellent resuscitation fluid for managing hemorrhagic shock states. We anticipate that SFHbNP will serve as a valuable alternative to RBCs in various clinical applications.

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One-Step Synthesis of AgNPs/MWCNTs Composites for Flexible Transparent Conductive Films

Jun Natsuki, Shinshu University, Japan

Plasmonic Carbon-Gold Hybrid Layer Integrated with Aligned Cellulose Aerogel for Efficient Solar-Driven Evaporation

Suji Lee, Kyung Hee University, South Korea

High Performance Lignocellulose Nanofiber-Derived Films for Efficient Light Management

Yuri Seo, Kyung Hee University, South Korea

Preparation of Artificial Lipid Lamellar Body Mimicking Giant Multilamellar Liposome and Its Skin Barrier Function Modulation Effect.

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Skin lipids are essential elements in maintaining the skin barrier function by reducing trans epidermal water loss (TEWL) through intercellular pathway and protect against external harmful substances penetration. However, various exogenous factors including exposure to UV radiation and toxic chemicals, as well as endogenous factors, such as chronological aging and skin disease can lead to changes in lipid composition and disturb their molecular arrangement. To recover its barrier function, previous studies have mostly focused on forming a hydrophobic liquid film to prevent temporal water evaporation from the skin surface and supply deficient lipid components, but they were not sufficient to maintain or restore the damaged barrier function of skin.

Therefore, in this study, GMLL, which mimic both lipid composition and the multi-lamellar structure of the skin barrier, was fabricated to restore the chemical properties and structural integrity of a damaged skin barrier. This is used to artificially simulate lipid lamellar bodies (LB) secreted from keratinocytes which supply structured lamellar lipids. This synthetic multilamellar body incorporated giant liposomes, having human stratum corneum lipid composition, was prepared by mixing lysophosphatidylcholine (Lyso-PC) with a thick, multilayered lipid film without a supporting polymer layer for hydration, by modifying the conventional film-assisted giant unilamellar liposome fabrication method.

Applying these GMLLs on surfactant-damaged pig skin demonstrated more effective restoration of the lipid arrangement in the damaged lipid membrane compared with liposomes that merely mimic lipid composition resulting in reduced TEWL and skin permeability.

3D Electron Tomography for Semiconductor Device Structure Analysis Yu-Lun Liu, Yu-Ju Lin, National Tsing Hua University, Taiwan

Quantum Neural Network for High Generalization Performance for Lubricant Property Prediction

Chanho Kim, Yonsei University, South Korea

Physics-Informed Neural Network Based Crystallization Modeling of NCM Precursor Recovery from Spent Batteries Gyeonggeun Park, Yonsei University, South Korea

AI-driven Catalyst Design for Photocatalytic Hydrogen Production: Techno-Economic and Regional Optimization

Juyoung Byun, Yonsei University, South Korea

Solution Plasma Synthesis of Nitrogen-doped Carbon Catalysts for Oxygen Reduction Reaction toward Li-Air Battery Takahiro Ishizaki, Shibaura Institute of Technology, Japan

A Review of Visible Light-Actived S-Scheme Heterojunction Photocatalysts for Environmental Pollutants Degradation

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Abstract

The rapid growth of industries and the rising global population in recent decades have exacerbated water shortages and pollution in many countries. To ensure the long-term sustainability of human society, there is an urgent need for environmentally friendly technologies and effective wastewater treatment processes. Among the various proposed solutions, semiconductor-based photocatalysis has emerged as a promising approach, owing to its ability to harness light irradiation and catalysts for the efficient degradation of harmful pollutants. However, single-phase semiconductor photocatalysts often suffer from rapid recombination of photogenerated electron/hole pairs and limited visible light absorption, resulting in low photocatalytic efficiency under visible light conditions. To address these drawbacks, heterojunction photocatalysts have been developed to suppress charge carrier recombination and enhance performance. Nonetheless, in conventional type-II staggered-gap heterojunctions, both photoexcited electrons and holes migrate to lower energy states, which reduces their oxidation and reduction capabilities compared with the original semiconductors. To overcome this limitation, S-scheme heterojunction photocatalysts-comprising a highoxidation-potential semiconductor and a high-reduction-potential semiconductor-have been proposed. This configuration retains the strong redox abilities of the constituent materials, enabling the generation of highly reactive oxygen species. As a result, S-scheme heterojunctions achieve not only efficient charge separation but also high reactivity and stability under visible light irradiation, making them particularly effective for degrading refractory pollutants in wastewater.

Key words: recombination, catalyst, visible-light irradiation, degradation, pollutant, S-scheme heterojunction photocatalyst

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Fabrication of Hierarchically Structured Polyethylene Naphtalate Composites With Noble Metal Nanoparticles for Tissue Engineering

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The development of micro- and nanopatterned and functionalized surfaces is lately undergoing extensive research for their intriguing multifunctional properties and wide variety of potential applications in either biomedical field, such as in tissue engineering, or optics and sensor fabrication. Simultaneously, there is a substantial surge in research of novel composite materials, by courtesy of discovering materials with new or improved properties and therefore further range of applications. Bringing this insight together, the combination of surface patterning and composite materials may lead to the creation of materials tailored to desired use.

In the presented study, we focused on fabrication of hierarchically structured polyethylene naphtalate (PEN) substrates/scaffolds enriched with gold and silver nanoparticles for use in tissue engineering. The substrates were prepared by simple few step method. First, the major groove micropattern was replicated by soft lithography onto polydimethylsiloxane (PDMS) master from commercially available optical discs (CDs, DVDs). This method was proven as an affordable and precise method of obtaining periodical patterns on large surface and with optimal dimensions for tissue engineering. Subsequently, the PDMS master was used as a stamp for hot-embossing onto PEN surfaces enhanced by sputtered thin metal layers (gold, silver). During the hot-embossing process, the non-continuous metal layers form nanoclusters and nanoparticles under the influence of the elevated temperatures and as such are then embedded into the polymer surface. Resulting substrates are therefore hierarchically structured, with pronounced metal nanoparticles superposed on larger microscale grooves. Formation of superposed secondary globular structures on the grooved PEN surface was confirmed by both scanning electron microscopy (SEM) and atomic force microscopy (AFM), as well as was the chemical composition by X-ray electron spectroscopy (XPS) and energy dispersive spectroscopy (EDS).

This desired structure significantly increased the surface area and roughness but also changes the optical behavior of the surface. The combination of changes in surface morphology, chemistry and wettability induced significant change in PEN antibacterial properties. PEN substrates enhanced by silver proved to have great antibacterial response against both gram-positive and gram-negative bacterial strains. The gold enriched surfaces have great potential for use in surface-enhanced Raman spectroscopy (SERS). Thanks to the aromatic nature of PEN, the composite surfaces are also excellent adepts for laser induction of tertial superposed structures – LIPSS (laser induced periodical surface structures) [1]. The successful surface patterning and noble metal enhancement of PEN surfaces thus shows promise in use for instance as antibacterial implant coatings or as supportive scaffolds for growth of muscle cells and tissues. The outcome of this research also contributes to improved comprehension of surface properties and interactions between structured polymer-metal composite surfaces and mammalian cells.

Acknowledgement: This work was supported by the Project OP JAK_Mebiosys, No CZ.02.01.01/00/22_008/0004634, of the Ministry of Education, Youth and Sports, which is co-funded by the European Union. References: 1. Kasálková, N. S.; Juřicová, V.; Rimpelová, S.; Fajstavr, D.; Frýdlová, B.; Kolská, Z.; Švorčík, V.; Slepička, P. LIPSS pattern induced by polymer surface instability for myoblast cell guidance. Polymer Degradation and Stability 2024, 221, 110667. DOI: https://doi.org/10.1016/j.polymdegradstab.2024.110667.

Generative Digital Twin Platform for Dry-Processed Electrode Design Jaejin Lim, Rakwhi Hong, Seungyeop Choi, Seung Wook Yang, Yong Min Lee Yonsei University, South Korea

Aluminum Nitride Ceramic-Coated Separators for Interfacial Stabilization of Lithium Metal Batteries Seungyeop Choi, Junhyeok Choi, Dongyoon Kang, Yong Min Lee Yonsei University, South Korea

Efficts of Perovskite Quantum Dots on photovoltaic and photocatalytic activities

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Perovskite quantum dots (QDs) are nano-scaled miniaturization of perovskite bulk crystals and are luminous materials with high luminescent quantum yields and narrow half-width optical properties similar to bulk crystals [1]. QDs described by CsPbX₃ shift an emission spectrum from 400 to 700 nm when X is converted into Cl, Br, and I ions. In this study, we report effects of adding green light-emitting CsPbBr₃ semiconductor nanoparticle on photovoltaic and photocatalytic systems.

The high performance of perovskite solar cells was achieved with the aid of an electron transport layer (ETL) and a hole transport layer. Perovskite cells were fabricated by coating carbon quantum dot on mesoTiO₂ ETL [2]. The manufactured mesoTiO₂/carbon dot-based devices reduced the pinholes of the perovskite film layer compared to mesoTiO₂-based devices and increased the average power conversion efficiency (PCE) of the device by 3%. The coating of carbon dot on mesoTiO₂ reduced carrier recombination, and fade-away X-ray diffraction spectra of perovskite film cracks showed the removal of perovskite components after spin coating of carbon dot on mesoTiO₂ ETL, indicating the improved device performance compared to mesoTiO₂ ETL due to the inhibition of non-radiative recombination. Thus, the electron injection from carbon dot improved electron transport between ETL and perovskite layers, resulting in high-quality perovskite cells by coating mesoTiO₂ ETL with carbon dots. The addition of carbon dot to N719 dye photosensitized solar cells was contributed by carbon dot-sensitized N719. When carbon dot was replaced with perovskite quantum dot, PCE increased by about 6%. These studies show that co-sensitization by fluorophore (perovskite quantum dot) and N719 is a viable approach to promote the efficiency of solar devices for energy generation.

Carbon neutrality is a global issue that scientists should prioritize. The purpose of research is to develop an optimal catalyst and reaction system that decomposes CO_2 and produces methanol, which is a raw material for fuels and chemicals. Especially, the challenge is to integrate perovskite quantum dots as photosensitizers [3]. The material has a synergistic effect on the photoconversion of CO_2 by directly approaching the catalytically active site (CuO). This improvement is due to energy transfer within the reaction system. The reaction system finally achieved the highest methanol yield (11.9 mmol/g (catalyst)).

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Defect Engineering of Inorganic Nanosheet-based Materials for Electrocatalytic Water Splitting

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The defect engineering of nanostructured materials has garnered significant research interest due to its utility in exploring high-performance energy-functional materials. The introduction of crystal vacancies into nanostructured material is found to be quite effective not only in tailoring the electronic and local structures but also in increasing the electrochemical activity. Since crystal defects can serve as efficient adsorption/reaction sites for ions, electrolytes, and catalysis reactants, the defect engineering can provide a versatile means to optimize the electrocatalyst functionalities of nanostructured materials. In this talk, I will present diverse examples of defect-engineered nanostructures along with the correlation between chemical bonding nature and energy functionalities. The various roles of crystal vacancies in optimizing the catalyst performances will be highlighted based on combined in situ/ex situ spectroscopic analyses.

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A Novel Wastewater Treatment Method Utilizing the Combination of Ultrasound and Plasma

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Granule-Induced Dry Processing for Accelerating Ion Transport in Thick-Film Electrodes for High-Energy-Density Lithium-Ion Batteries

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Thick-film electrodes have attracted significant attention as a viable strategy to simultaneously improve the energy density and cost-effectiveness of lithium-ion batteries. Among various fabrication approaches, dry processing, which is a solvent-free method for electrode manufacturing, has emerged as a promising route for producing high-performance, low-cost electrodes. However, the strong shear forces and friction generated during dry processing can mechanically damage active materials, accelerating degradation and reducing electrode porosity. In addition, the poor dispersibility of PTFE binder often deteriorates the electrode microstructure and exacerbates ionic resistance. Since thick-film electrodes inherently suffer from high resistance, overcoming these limitations is essential to fully realize the potential of dry processing for such electrodes.

In this work, we propose a granule-induced dry processing method that enables the fabrication of low-resistance thick-film electrodes through the formation of composite granules composed of active material, conductive additive, and binder. Granule formation mitigates mechanical damage to the active material during electrode sheet fabrication, while the pre-fibrillation of PTFE binder during granulation yields a uniform and robust binder network. As a result, active material degradation and side reactions at high voltage are minimized, and the resulting electrodes possess a stable, ion-conductive microstructure. Furthermore, the homogeneous binder distribution effectively accommodates volume changes in high-nickel cathodes, ensuring long-term cycling stability. The electrodes fabricated using this method exhibit stable performance even under ultra-high loading conditions exceeding 8 mAh cm⁻², and the feasibility of the process is further confirmed through full-cell demonstrations. This study provides a practical route and new insights into the scalable fabrication of high-energy-density thick-film electrodes via dry processing.

Proton conduction mechanism in a material consisting of packed acids for high proton conductivity with low humidity conditions

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The proton conducting membrane has been the focus of attention as an indispensable component for polymer electrolyte fuel cell. General proton conduction mechanisms require water movements, resulting in a fatal drawback of proton conducting electrolytes; proton conductivity highly depends on relative humidity (RH) and severely decreases at low RH. Instead, the packedacid mechanism has been proposed as a proton conduction mechanism in a material consisting of packed acids [1]. In the packed-acid mechanism, proton conducts by acid-acid interaction without help of water movements. The mechanism has a potential to improve its dependency on RH. In this presentation, I propose a material design to cause the packed-acid mechanism dominantly using ab initio calculations, and show materials synthesized according to the design. First, I performed DFT calculations using SIESTA 2.0.1 software package. The electronic structure is represented with GGA using the RPBE functional. I have calculated several models composed of water molecules and various acid groups with changing acid density. Optimized structures were analyzed to find important factors for the packedacid mechanism. I investigated suitable types of acid groups and the optimal density for acids in order to facilitate packed-acid mechanism effectively [2]. The calculation results were utilized for experiments as a material design. The material which possesses the optimal acid group was synthesized. Details of experiments will be presented at the conference. As the acid density increases, the material exhibited lower dependence on RH, which reflects the properties of the packed-acid mechanism. Especially, the material with high acid density showed an extremely low RH dependence; its proton conductivity at 95% RH decreased to 2/3 at 40% RH while Nafion decreases to 1/20 its value under the same conditions [3]. I will present the optimal acid group, the preferable acid density, and the method to prepare the electrolyte membrane that can induce the packed-acid mechanism dominantly [4]. Keywords: Proton conductivity at low humidity condition, electrolyte membrane, DFT calculation [1] Ogawa, T., et al., Chem. Sci. 2014, 5 (12), 4878-4887 [2] Ogawa, T., et al., Phys. Chem. Chem. Phys. 2021, 23 (41), 23778-23786 [3] Ogawa, T., et al., Mater. Chem. Front. 2022, 6 (21), 3271-3278 [4] Ogawa, T., et al., Int. J. Hydrog. Energy 2023, 48 (80), 31337-31349.

Sustainable Synthesis of High-Performance Ni/Co-AC Pseudocapacitor Electrodes from Recycled Battery and Biomass Waste

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The global volume of spent lithium-ion and nickel-metal hydride (NiMH) batteries has surged over the past decade, driven by the rising demand for energy storage devices. Transforming these waste materials into high-performance, sustainable resources is critical for addressing supply-demand challenges and promoting environmental sustainability. Supercapacitors, valued for their high power density, fast charging, and long cycle life, are limited by low energy density and high production costs. In particular, pseudocapacitors rely on battery-like electrode materials, such as virgin nickel (Ni) and cobalt (Co), leading to environmental and economic burdens akin to battery production. Current research lacks scalable, sustainable methods to produce high-performance pseudocapacitor electrodes from recycled materials.

This study presents a sustainable strategy for synthesizing high-performance supercapacitor electrodes using recycled materials. Nickel (Ni) and cobalt (Co) are recovered from spent NiMH batteries, while activated carbon (AC) is derived from lignosulfate, a biomass by-product. A novel AC-assisted precipitation and hydrothermal treatment process is employed, where AC serves as a nucleation site to facilitate Ni/Co precursor formation, streamlining metal recovery and electrode synthesis into a single-step process. This co-doping approach anchors Ni and Co into the carbon framework, enhancing electrical conductivity and pseudocapacitive behavior. The resulting Ni/Co-AC composite leverages AC's high surface area and Ni/Co's redox properties, enabling direct use of it as supercapacitor electrode active materials without additional processing. Our work will optimize the recycling process, Ni/Co ratio, and AC content to maximize the derived pseudocapacitor's performance.

Impact of Acetic Acid and Flux Residues on ITO Corrosion in Heterojunction Silicon Solar Cells

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The global solar photovoltaic (PV) market is rapidly expanding, with projections estimating a capacity of 11.6 TW by 2050. Among advanced silicon-based solar technologies, heterojunction technology (HJT) solar cells have emerged as a promising candidate due to their record-high power conversion efficiency (exceeding 26%) and suitability for bifacial operation. The high performance of HJT devices stems from their unique multilayer structure: thin hydrogenated amorphous silicon layers provide excellent surface passivation, while indium tin oxide (ITO) transparent conductive oxide layers serve as both antireflection coatings and efficient lateral current collectors. However, despite their efficiency advantage, the long-term reliability of HJT solar cells remains a key concern, primarily due to corrosion and degradation of ITO layers under field-relevant stress conditions.

In this study, we investigated two major degradation pathways that compromise ITO stability in HJT cells. First, encapsulant-induced acid formation was systematically studied using ethylene vinyl acetate (EVA), polyolefin elastomer (POE), and a sandwich-structured EVA-POE-EVA (EPE) encapsulant. Accelerated pressure cooker tests revealed that EVA and EPE generate acetic acid at elevated temperatures above 120 °C, conditions that can occur locally during hotspot formation. The resulting acidic environment, with pH values dropping below 3.5, was shown to selectively corrode the rear-side ITO. Structural and compositional analyses indicated that the rear ITO contains additional crystalline phases, which makes it more vulnerable to dissolution. Corrosion manifested as severe increases in sheet resistance and was demonstrated by electroluminescence imaging, where darkening regions emerged due to loss of current conductivity.

Second, the role of solder flux residues from interconnection processes was examined as an additional source of ITO degradation. Commercial fluxes containing organic acids were applied to HJT precursors and full modules. Even after lamination, flux residues persisted and became highly corrosive under damp heat conditions. Again, corrosion predominantly affected the rear ITO, leading to substantial increases in resistivity. Comparative testing of different flux chemistries demonstrated that flux acidity and halogen content strongly influenced the extent of degradation. Importantly, implementing a simple hot-air drying step prior to lamination effectively minimized flux-induced corrosion, extending the durability of HJT cells under accelerated stress testing.

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