DAY–1, 9 NOVEMBER, 2026

Welcome Reception and Opening Remarks

DAY–2, 10 NOVEMBER, 2026

Session: Energy and Environmental Materials

Boron-doped Diamond Powder-packed Electrolysis Flow Cell for Water Treatment

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Conductive boron-doped diamond (BDD) electrodes are promising candidates for electrolytic water treatment applications owing to their excellent durability under high-potential conditions in aqueous solutions and their ability to efficiently generate hydroxyl (OH) radicals, which can ultimately decompose organic matter into CO2. We developed an electrolytic flow cell with a BDD powder (BDDP)-packed bed as the anode and investigated its application in water treatment [1]. The BDDP-packed flow cell forces water to pass through narrow voids within the packed bed, increasing the contact efficiency with OH radicals present on or near the electrode surfaces, thereby enabling efficient organic matter decomposition. In this study, we investigated the effects of parameters such as packed-bed dimension, BDDP amount, and electrolysis voltage on the electrolytic oxidative decomposition of organic matter using a BDDP-packed flow cell. BDDP (particle size: 40–60 µm) was prepared by growing a conductive BDD layer onto the surface of(insulating) diamond powder substrates using the microwave plasma-assisted CVD method. Methylene blue (MB)was used as a model organic pollutant, and electrolysis was performed on a solution containing 50 µM MB and 1 MNa_2SO_4. We fabricated BDDP-packed flow cells with packed-bed diameters of 1.0, 1.5, and 2.0 cm (designated as Types A, B, and C, respectively) and compared their electrolytic characteristics. The electrolysis of an MB solution was conducted using cells (BDDP amount of 10 g) of varying diameters at voltages of 10, 30, 45, and 60 V. Under all conditions, the MB concentration decreased exponentially with time. In the Type A cell (packed bed diameter: 1.0 cm), the MB degradation rate showed almost no dependence on the electrolysis voltage. In contrast, for Type B (diameter: 1.5 cm) and Type C (diameter: 2.0 cm) cells, the degradation rate increased with the electrolysis voltage. Because the BDDP amount was fixed at 10 g, the height of the packed bed varied depending on the flow cell type. In the Type A cell, the small diameter and large height of the packed bed resulted in a high pressure drop and poor flow; consequently, oxygen bubbles generated during electrolysis likely accumulated, thereby inhibiting MB degradation. Conversely, in the Type B and C cells, which featured larger diameters and lower packed-bed heights, the flow was smoother, allowing an increase in the MB degradation rate with higher electrolysis voltages. These findings indicate that minimizing the pressure drop and bubble accumulation is crucial for achieving efficient electrolysis in BDDP-packed flow cells.

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Efficient Low-Voltage CO 2 -to-CO Electrolysis Using a Polymer-Coupled Mn Molecular Catalyst

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Electrochemical CO 2 reduction to CO is a promising approach for renewable carbon conversion. However, practical implementation remains hindered by the relatively high cell voltages required for selective CO production. Although considerable effort has been devoted to increasing current density, lowering the operating voltage is equally important for improving the energy efficiency of CO 2 electrolysis. Here, we demonstrate low-voltage CO 2 -to-CO electrolysis using a polymer-coupled Mn molecular catalyst in a membrane electrode assembly (MEA). The cathode employs a non-planar Mn(I) bipyridine complex bearing pyrrolyl-functionalized ligands. Oxidative polymerization of the pyrrole groups forms a conductive polypyrrole- linked network, providing efficient electronic coupling between the molecular catalyst and the carbon support in the gas-diffusion electrode. Combined with a Ni-doped β-FeOOH anode for water oxidation and an anion-exchange membrane, the MEA achieves a CO Faradaic efficiency above 94% at a cell voltage of only 1.35 V in 1 M KOH. Under identical conditions, the Mn polymer catalyst delivers CO partial current densities comparable to those of Ag and planar molecular catalysts while operating at substantially lower cell voltages. Operando surface-enhanced Raman spectroscopy together with density functional theory calculations suggests that electron-withdrawing substituents stabilize a one-electron-reduced intermediate and promote a reaction pathway distinct from that of conventional Mn(bpy)(CO) 3 Br catalysts. The polymer framework further facilitates charge delocalization, while phenol incorporated in the catalyst layer promotes CO 2 coordination without stoichiometric consumption. The intrinsically low operating voltage enables direct coupling of the electrolyzer to a three-series crystalline silicon photovoltaic unit without external power conditioning. Under simulated solar illumination, the photovoltaic output matches the electrolyzer load at approximately 1.39 V, enabling stable solar-driven CO 2 electrolysis with CO selectivity above 95% for 50 h. The apparent solar-to-CO conversion efficiency reaches 20.4% over the first 12 h and remains at 20.0% over 50 h under alkaline conditions, where the contribution of the pH gradient is not included in the efficiency definition. This direct photovoltaic coupling serves as a validation of the low-voltage electrochemical design and demonstrates the compatibility of voltage-oriented molecular catalysis with cost- effective silicon photovoltaics. ReferenceK. Sekizawa et al., ChemRxiv, DOI: 10.26434/chemrxiv-2024-brj46. Acknowledgements This work was supported by the Ministry of the Environment, Government of Japan, and the Uncharted Territory Challenge 2050 program of NEDO, Japan.

Beyond PEO: Redesigning Polymer Electrolytes for Scalable Solid-State Batteries

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All-solid-state batteries (ASSBs) offer a promising route toward safer and higher-energy-density energystorage, yet their practical implementation remains constrained by insufficient room-temperature ion transport, unstable solid–solid interfaces, high stack-pressure requirements, and limited compatibility with scalable electrode and cell manufacturing. Polymer electrolytes are attractive because of their synthetic versatility, mechanical compliance, and potential integration with established lithium-ion battery processes. However, conventional polymer electrolytes remain dominated by polyethylene oxide (PEO), whose crystallinity, limited salt dissociation, segmental-motion-dependent Li+ transport, and low Li+ transference number impose intrinsic limitations on electrochemical performance and practical cell integration. This presentation introduces a “Beyond PEO” framework that redesigns polymer electrolytes as integrated ion-transport, mechanical, interfacial, and manufacturing architectures. Rather than treating the polymer merely as a passive matrix for dissolving lithium salts, this approach controls entropy, supramolecular organization, dynamic bonding, and electrolyte composition to establish designed Li+-transport pathways while simultaneously addressing mechanical durability and electrode integration. Conflicting-entropy-driven zwitterionic polymer electrolytes illustrate how molecular organization can promote salt dissociation and generate Li+-transport environments beyond conventional segmental-motion- controlled conduction. The competing interactions among zwitterions, lithium salts, and polymer chains suppress unfavorable ordering while creating ionically organized domains, enabling ambient-temperature operation of pouch- type ASSBs. Ionic dimer elastomers extend this concept by introducing dynamic ionic crosslinks that combine ion mobility with mechanical resilience. Their reversible bonding networks accommodate interfacial deformation and maintain electrolyte integrity without severely restricting Li+ transport. Building on these molecular design principles, monomer-in-salt polymer catholytes address scalability at the electrode-processing and cell-manufacturing levels. In this inverted architecture, concentrated lithium salts constitute the primary ion-transport medium, while a relatively small fraction of polymerizable monomers provides structural stabilization through in situ polymerization. Direct formation of the catholyte within dry-processed composite electrodes eliminates conventional solvent-based catholyte processing and produces compositionally uniform, mechanically integrated, and ionically continuous networks. This strategy enables intimate contact among active materials, conductive additives, and the solid electrolyte, supporting their implementation in Ah-class pouch cells. The resulting polymer-electrolyte architectures also reduce dependence on high external stack pressure by maintaining conformal electrolyte–electrode interfaces and continuous ion-transport pathways during cell operation. More broadly, solvent-free processing, in situ network formation, compatibility with dry electrodes, and integration with existing battery-manufacturing infrastructure provide practical routes from molecular electrolyte design to scalable cell fabrication. These studies establish “Beyond PEO” as a general framework for redesigning polymer electrolytes across multiple length scales from ion coordination and supramolecular structure to composite-electrode processing and pouch-cell integration. By treating ion transport, mechanics, interfaces, and manufacturability as interconnected design variables, this approach provides a pathway toward robust, low-pressure, and scalable polymer-based solid-state batteries.

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From Chemical Solution Processes to Functional Nanostructured Thin Films for Energy and Environmental Applications

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Functional thin films or coatings, with thickness ranging from nanometres to micrometres, are playing an important role in daily life. Recently, the demand for robust, low cost and friendly-environmental functional nanocomposite thin films with high transparency for window saving-energy applications or with strong antibacterial properties against biofilm is strongly increasing. Moreover, the use of chemical solution disposition (CSD) processes is highly desirable in order to reduce the cost and waste. This presentation will summarize our recent works on the synthesis of functional nanostructured nanocomposite thin films based on metal atom clusters by CSD processes (spin- coating, dip-coating and/or electrophoretic deposition).[1-3] 1) N.T.K. Nguyen et al., A review on functional nanoarchitectonics nanocomposites based on octahedral metal atom clusters (Nb 6 , Mo 6 , Ta 6 , W 6 , Re 6): inorganic 0D and 2D powders and films, Sci. Technol. Adv. Mater., 2022, 23(1),547. 2) K. Kirakci et al., Electrophoretically deposited layers of octahedral molybdenum cluster complexes: a promising coating for mitigation of pathogenic bacterial biofilms under blue light, ACS Appl Mater Interfaces, 2020, 12(47), 52492. 3) N.T.K. Nguyen et al., Molybdenum Nanoclusters-Functionalized Porous TiO 2 Inverse Opal Layers for Light- Activated Inhibition of S. aureus Biofilms, ACS Appl. Nano Mater. 2026, 9, 4462.

Bifunctional Metal-Organic Frameworks for Electrochemical Energy Storage and Green Hydrogen Generation

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Metal-organic frameworks (MOFs) and their derivatives have attracted significant interest in clean energy fields due to their high specific surface area, tunable pore structures, and uniformly dispersed active sites. In this work, we demonstrate the development of a highly efficient, multifunctional MOF-based material capable of serving as a heterogeneous catalyst for thermal ammonia decomposition, as well as a dual-functional electrode for electrochemical water splitting and supercapacitors. For hydrogen production via thermal NH 3 cracking, the robust MOF-derived architecture provides excellent thermal stability and highly exposed active centers, facilitating efficient nitrogen-nitrogen coupling and hydrogen desorption at elevated temperatures. Meanwhile, the rich porosity and tailored electronic structure of the material significantly enhance its electrochemical performance. It exhibits promising electrocatalytic activity for water splitting with lowered overpotentials for both hydrogen and oxygen evolution reactions, while simultaneously delivering a high specific capacitance and exceptional cycling stability as a supercapacitor electrode. This study highlights the immense versatility of rationally designed MOFs in bridging thermal catalysis and electrochemical energy technologies.

Engineering Iron Oxides: The Roles of Metal Elements in Solid Solutions and Phase Separation

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Iron oxides are composed of the abundantly available resource “iron”. They are relatively low-cost and easy to source, and recycling methods are well established, making them suitable for a circular economy as well as a sustainable society. As oxidation progresses, iron undergoes phase transitions in the order of wüstite (FeO), magnetite (Fe 3 O 4), maghemite (γ-Fe 2 O 3), and hematite (α-Fe 2 O 3), exhibiting properties such as ferrimagnetism or semiconducting behavior depending on the degree of oxidation. Specifically, magnetite and maghemite exhibit ferrimagnetism, while maghemite and hematite are semiconductors with optical absorption edges in the visible spectrum. Magnetite, which exhibits the properties of a half-metal, shows metallic behavior in the up-spin state and possesses a narrow-gap semiconductor band structure in the down-spin state. The electrical resistivity dynamically varies, ranging from the relatively low resistivity of magnetite to the relatively high resistivity of hematite. Utilizing such characteristics, considerable efforts have been made in the fields of magnetics, optics, electronics, and electrochemistry. On the other hand, iron oxide presents challenges such as thermal instability, short lifetimes of generated electrons, and complex fabrication processes. This presentation provides an overview of enhancing functionalities by either “solid solution” or “phase separation” between specific metal elements and iron oxides. In the materials design of “solid solution”, the addition of Si allows the metastable phase of maghemite to exhibit thermal stability even at relatively high temperatures, 1 whereas the addition of Ge enables magnetite to exhibit oxidation resistance. 2-5 In addition, through these heat treatments in air, iron oxide self-forms a unique

heterostructure. This distinctive structure consists of hematite with a randomly uneven surface formed relatively thinly, while the internal phase is composed of heat-resistant spinel materials, magnetite or maghemite. Moreover, this unique structure has been confirmed as an intrinsic behavior that appears regardless of whether the material is in thin film, sintered body, or powder form. As an application example in powder form, it is effective as a visible light- responsive photocatalyst. In materials design based on “phase separation”, the addition of platinum (Pt) results in nanocomposite thin films with iron oxides, in which Pt is uniformly dispersed in magnetite and hematite at sizes of a few nanometers. 6 Moreover, because their work function is larger than the electron affinity of magnetite and hematite, Pt can effectively capture electrons generated in iron oxides under light irradiation. For example, when magnetite is irradiated with mid-infrared light, the photodetection characteristics can be enhanced by effectively capturing thecharge carriers generated in the magnetite with Pt nanoparticles. On the other hand, when Cu or Mg is added to hematite during film preparation, a reductive phase transition to metastable maghemite occurs in one-step. In this case, the added elements are phase-separated and exist within the thin film. This is essentially a unique processing method. 7,8 Furthermore, Cu is an element that exhibits surface plasmon resonance, and the formation of a nanocomposite with maghemite can also be expected to enhance optical absorption. Therefore, by selectively adding specific elements to induce either “solid solution” or “phase separation”, it is possible to enhance the functionality of iron oxides.

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Multidimensional Hierarchical Metal nanoparticles/two-dimensional Transition Metal Dichalcogenide Nanocomposites as Electrocatalysts for Efficient Hydrogen Evolution Reaction

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Phase- and Interface-engineering of two-dimensional (2D) transition-metal dichalcogenide (TMDs) provides an effective approach to improving their insensitive semiconducting phase for hydrogen evolution reaction (HER) performances. Herein, we report a hybrid strategy of a top- down plasma-exfoliation first step and a bottom-up hydrothermal-growth second step for fabricating metal nanoparticles/two-dimensional transition metal dichalcogenide nanocomposites as electrocatalysts for hydrogen evolution reaction. There are two case studies presented: (i) selectively ruthenium nanoparticles (Ru NPs) decoration on WS 2 nanosheets fabricated with plasma exfoliation and in situ polyol-reduction as electrocatalysts for enhanced HER and (ii) homogeneous ruthenium nanoparticles decoration on 1T/2H WSe 2 nanosheets for HER. In the first case, the dispersion of Ru NP near WS_2 NS edges is predicted with a much larger binding energy on edges than on basal planes (-11.01 vs. -8.41 eV) with density function theory (DFT) that also show lower Gibbs free energies of hydrogen adsorption ΔG H (-0.21 eV) at WS_2@Ru3 edge sites. WS_2@Ru3 (6 wt% Ru NP) sample shows optimal HER activity with an overpotential of 83 mV at 10 mA cm^{-2} and a Tafel slope of 56 mV dec^{-1}, smaller than those of pristine WS_2 NS (283 mV and 146 mV dec^{-1}), and retains excellent stability after 1,000 cycles. The second case involves conducting (1T) and semiconducting (2H)phase presented 2D WSe 2 nanosheets (WSe 2 NS) with rather uniform decroration of Ru NPs (~3nm) occurring because the Ru NPs have offset binding energy values on the basal plane and Se edge (−12.93 and −11.88 eV for 1T phase, and are −7.52 and −10.03 eV for 2H phase, respectively), and induces ΔG H values closer to zero. Electrochemical measurements reveal that the optimized incorporation of 7.5 wt% Ru NPs in WSe 2 NS, Ru7.5–1T/2H WSe 2 NS nanocomposite, catalyst delivers a strong HER performance with a low overpotential of 154 mV at 10 mA cm -2 and a small Tafel slope of 58 mV dec -1 , as compared to 358 mV and 101 mV dec -1

Role of Oxygen in Enhancing Catalytic Activity for Ammonia Synthesis: The Case of Ru/CaH 2−2x O x

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In the field of NH 3 synthesis heterogeneous catalysis, oxygen is traditionally regarded as a "poison" or a detrimental species due to its strong electron-withdrawing nature. In ammonia synthesis over ruthenium (Ru) catalysts, electronic promoters are typically required to donate electrons to Ru to facilitate the dissociation of the strong N≡N bond. Because oxygen tends to withdraw electrons, its presence is conventionally thought to suppress catalytic activity by increasing activation barriers. However, this study presents a counter-intuitive and remarkable finding: the intentional and controlled incorporation of oxygen into a Ru/CaH 2 catalyst does not hinder, but instead significantly enhances, the ammonia synthesis rate under mild conditions. We investigated the catalytic performance of Ru-loaded calcium oxyhydride (Ru/CaH 2−2x O x) with varying oxygen contents (x = 0.00–0.44). The reaction rate at 300 °C and 0.1 MPa exhibited a distinct volcano-type dependence on the oxygen content, peaking at x ≈ 0.29. At this optimal concentration, the ammonia synthesis rate (1510.8 μmol h^{-1} g^{-1}) was approximately twice that of the low-oxygen variant, and the

apparent activation energy was reduced to its minimum (59 kJ mol^{-1}). This enhancement is paradoxical because oxygen is inherently more electronegative than hydrogen or nitrogen. The origin of this "oxygen-induced enhancement" was elucidated through structural and kinetic analyses. X-ray diffraction (XRD) and density functional theory (DFT) calculations revealed that oxygen incorporation triggers a contraction of the CaH 2 lattice by inducing the formation of hydrogen vacancies (VH). They create localized electron states with an exceptionally low work function (2.7 eV), which is significantly lower than that of pure CaH 2 (approx. 5.2 eV). Consequently, these oxygen-induced vacancies transform the support into a potent electron donor, facilitating stronger electron transfer to the Ru nanoparticles. Furthermore, we demonstrates that oxygen plays a crucial role in mitigating "hydrogen poisoning." At lower temperatures (below 350 °C), Ru catalysts are often deactivated by strongly adsorbed hydrogen atoms that block nitrogen activation sites. Our kinetic modeling shows that the presence of oxygen-induced vacancies increases the support's capacity for hydrogen absorption, effectively keeping the Ru surface clean for nitrogen dissociation. This shifts the rate-determining step from N 2 dissociation to subsequent hydrogenation (NH* or NH 2 * formation), as evidenced by the shift in H 2 reaction orders from -0.85 to +0.05. By challenging the conventional view that oxygen is a catalytic inhibitor, this work provides a new design principle: using controlled oxidation to tune vacancy chemistry and maximize the performance of oxyhydride catalysts for sustainable energy applications. On the day of the presentation, I will also discuss other catalysts whose activity is actually enhanced by oxygen.

Machine-Learning Molecular Dynamics with Born Effective Charges for Predicting Dielectric and Ionic Properties of Complex Materials

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The response of materials to applied electric fields is fundamental to energy storage, electronic devices, and information technology, and is closely related to dielectric response, structural and phase transitions, ferroelectricity, and ion transport. Although density functional perturbation theory (DFPT) provides an accurate framework for calculating dielectric properties, its high computational cost limits its application to large-scale systems and finite- temperature simulations. We have developed a hybrid equivariant graph neural network (h-EGCNN) framework that predicts both the Born effective charge (BEC) tensor and interatomic force field under external electric fields [1,2]. The model combines Equivar, trained using DFPT data to predict BEC tensors, with MACE, trained using ab-initio molecular dynamics (AIMD) data to predict interatomic forces. This hybrid architecture improves computational efficiency and enables large-scale molecular dynamics (MD) simulations while retaining the physically grounded and non-arbitrary nature of BECs, which naturally account for charge fluctuations arising from local atomic environments. We first established the methodology using $CaTiO_3$, an important dielectric material with a relatively high dielectric constant and weak temperature dependence near room temperature. Large-scale MD simulations of a 640- atom system over 0-1700 K enabled evaluation of polarization and dielectric tensors from atomic displacements and BEC tensors under applied electric fields. Careful optimization of the sampling protocol, including treatment of the observed nonlinear polarization–electric-field relationship, yielded temperature-dependent dielectric properties, including anisotropy and the orthorhombic–tetragonal–cubic phase transitions. The low-temperature dielectric constants converged toward DFPT results, while analysis of local structures,

phonon frequencies, and BECs revealed microscopic origins of the phase transitions. The h-EGCNN framework was further applied to $BaTiO_3$, where machine-learning MD reproduced the ferroelectric-paraelectric Curie temperature of 380–385 K, close to the experimental range of 393–403 K, and enabled investigation of ferroelectric polarization and energy barriers. In addition, BEC-based nonequilibrium MD was used to evaluate ionic conductivity in the solid electrolyte $Li_{10}GeP_2S_{12}$[3]. Unlike fixed charge often used in conventional classical molecular dynamics, BEC is non- arbitrarily defined depending on the actual electronic response. The resulting conductivities were consistent with equilibrium MD using the Green–Kubo formalism while achieving faster convergence. These results demonstrate that h-EGCNN provides a versatile, scalable, and physically interpretable framework for quantitatively describing dielectric and ionic responses, including charge fluctuations, local structural variations, and correlations that are essential in complex materials.

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Digital Twin-Guided Materials and Electrode Design for High-Energy-Density Rechargeable Batteries

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High-energy-density rechargeable batteries are increasingly governed not only by the intrinsic properties of active materials but also by electrode microstructure, processing history, interfacial contact, and coupled ion/electron transport pathways. As battery electrodes move toward higher areal loading, higher density, reduced porosity, dry processing, and solid-state configurations, local microstructural heterogeneity becomes a critical factor determining practical energy density, rate capability, and long-term stability. Therefore, a quantitative framework that connects materials, processing, microstructure, and electrochemical performance is essential for rational battery design. In this talk, I will present our recent efforts in digital twin-guided materials and electrode design for high- energy-density rechargeable batteries. By integrating advanced structural characterization with three-dimensional, microstructure-resolved simulations, digital twin models enable direct quantification of key structural and transport descriptors, including porosity, tortuosity, particle connectivity, conductive-network formation, interfacial contact area, and effective ionic/electronic conductivity. These descriptors correlate with electrochemical polarization, reaction heterogeneity, rate performance, and degradation behavior, providing mechanistic insight beyond conventional cell-level measurements. Representative examples will include virtual calendering of composite electrodes, dry-processed ultra-high- active-content cathodes based on single-crystalline Ni-rich oxides, separator microstructure modeling, and interfacial design for solid-state battery components. These studies demonstrate how digital twins can identify transport bottlenecks, predict process–structure–property relationships, and guide electrode architectures that simultaneously improve energy density, power capability, and mechanical robustness. Overall, digital twin battery modeling provides a predictive and physically grounded platform for accelerating the development of next-

generation rechargeable batteries. By bridging materials innovation, electrode processing, and microstructure-level simulation, this approach offers a powerful design strategy for future lithium-on and all-solid-state battery systems.References

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Metal-Organic Carboxylates: From Hydrated Ion Conductors to Heterometallic Cluster Assemblies

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Organic carboxylates are fundamental building units for constructing coordination and hydrogen-bonded frameworks in supramolecular chemistry. Discrete metal complexes bearing non-coordinating carboxy groups, referred to as metal-organic carboxylates (MOCs), have attracted increasing attention as alternatives to conventional organic carboxylates because of their facile synthesis, structural diversity, and additional functions derived from transition-metal centers [1]. Inspired by the historically important Cu 14 cluster with D-penicillamine, the first MOC [2], we have developed a variety of metallosupramolecular aggregates based on amino-acid-derived MOCs [1,3]. One representative example is the octanuclear complex anion [Rh 4 Zn 4 (L-cys) 12 O] 6– ([1] 6–), which is a MOC having 12 COO - groups [3]. Its potassium salt, K 6 [1]·nH 2 O, exhibits room-temperature superionic conductivity through the migration of hydrated K+ ions. This material is mechanically soft, requires no high-temperature sintering, and retains high ionic conductivity at low temperatures. We have also extended this MOC chemistry to the synthesis oflanthanide cubane clusters. In this talk, I will describe the development of hydrated ion conductors based on MOCs and the extension of this chemistry to the controlled synthesis and assembly of heterometallic clusters. [1] N. Yoshinari, T. Konno, Coord. Chem. Rev., 2023, 474, 214850(1-39). [2] P. J. M. W. L. Birker and H. C. Freeman, J. Am. Chem. Soc. 1977, 99, 6890-6899; N. Yoshinari, K. Tatsumi, A. Igashira-Kamiyama, T. Konno, Chem. Eur. J. 2010, 16, 14252-14255. [3] N. Yoshinari, S. Yamashita, Y. Fukuda, Y. Nakazawa, T. Konno, Chem. Sci. 2019, 10, 587-593; R. Sakamoto, K. Nakamoto, A. Inoishi, M. Ito, N. Yoshinari, T. Konno, Y. Hara, T. Fujii, S. Okada, Chem. Asian. J. 2025, e202401781. N. Yoshinari, N. Meundaeng, H. Tabe, Y. Yamada, S. Yamashita, Y. Nakazawa, T. Konno, Angew. Chem. Int. Ed. 2020, 59, 18048-18053; S. Thammakan, N. Yoshinari, M. Tsuchikawa, A. Rujiwatra, T. Konno, Inorg. Chem., 2024, 63, 6239-6247; M. Kouno, T. Konno, N. Kuwamura, T. Kojima, S. Takamuku, S. Nishio, N. Yoshinari, Chem. Commun. 2026, DOI: 10.1039/d6cc03160a.

Development of Cost-Effective and High-Energy Cathodes for Next-Generation Rechargeable Battery

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Iron oxide-based materials are attractive cathodes due to their earth-abundant nature. There have been efforts made for a long time to utilize Fe4+/Fe3+ redox reactions at cathodes. Even in well-known alkali iron binary oxides such as LiFeO2 and NaFeO2, the utilization of Fe4+/Fe3+ one-electron redox is still challenging; excess oxidation leads to O2 evolution. Utilization of anionic oxygen redox in solids is a well-known strategy to achieve large reversible capacity, while large voltage hysteresis due to instability at the charged phase, i.e., the oxidized oxygen species, remains a critical issue.Herein, we introduce a new material of Na-Fe binary oxides, Na5FeO4, a thermodynamically stable phase in the Na- Fe-O phase diagram, for a sodium-ion battery cathode. The sodium-superrich Na5FeO4 is composed of tetrahedral FeO4 units, which is different from NaFeO2 (composed of octahedral FeO6 units). It delivers a two-electron redox reaction to achieve a high reversible capacity of 228 mAh g–1. X-ray absorption spectroscopy suggests that during the two-electron redox, a cationic Fe5+/Fe3+ redox with no O2 evolution proceeds, holding the tetrahedral FeO4 local structure.

Scalable Ternary-Solvent Growth of Ultrathin 2D Perovskite Crystals for Custom Optoelectronic Functionalities

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Department of Materials Science and Engineering, Faculty of Engineering, Monash University, Clayton, Victoria, Australia 3800 Solution-phase synthesis of monolayer hybrid organic–inorganic perovskites (A 2 MX 4) is fundamentally limited by rapid out-of-plane growth and aggregation, typically restricting flakes to small lateral dimensions. Here, we present a steric-engineering ternary-solvent growth strategy that suppresses out-of-plane crystal stacking and enables the synthesis of laterally extended monolayer and few-layer A 2 MX 4 crystals with surface areas exceeding 1000 µm 2 . By employing long-chain alcohol cosolvents combined with long-chain amine additives, secondary solvation environments are reorganized to prolong edge-mediated precursor transport during annealing. This platform demonstrates broad compositional universality across various organic cations, metal centers, and halides. The exceptionally large lateral dimensions allow direct, solvent-free electrical contact fabrication via physical shadow masking, bypassing chemical damage inherent to conventional lithography. Planar devices fabricated from ultrathin channels demonstrate diverse, composition-dependent optoelectronic behavior: PEA 2 PbI 4 channels yield ultra-low dark currents, and enhanced volume-normalized photosensitivity; conversely, lead-free PEA 2 MnCl 4 devices exhibit reproducible negative photoconductance driven by localized Mn-centered excitation and defect-assisted photogating. Together, these results establish steric solvation control as a general paradigm for synthesizing scalable 2D hybrid perovskite monolayers and exploring tailored metal-halide optoelectronic phenomena.

Hydrophobic Modification of MOF-based Photocatalysts for H2O2 Production

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Hydrogen peroxide (H2O2) has attracted much attention as an eco-friendly oxidant and liquid fuel [1-3]. Metal-organic frameworks (MOFs) are promising candidates for photocatalyst for H2O2 production because of their unlimited designflexibility [2-7]. The efficiency of H2O2 production in pure water has suffered from low O2 solubility in aqueous solution and difficult-to-inhibit H2O2 decomposition. In this work, we focus on hydrophobization of MOF photocatalysts to overcome the above challenges. We demonstrate that the hydrophobic modification of Zr-MOF significantly accelerates photocatalytic H2O2 production from O2 and H2O under visible-light irradiation [8]. Zr-MOF (Zr-TCPP) was synthesized using a solvothermal method with a high concentration of formic acid in DMF solution at 120 °C for 3 days. Perfluoroalkylation of Zr-TCPP was conducted by mixing with an acetonitrile solution containing a perfluoroalkyl carboxylic acid at 60 °C for 1 h. The series of perfluoroalkylated Zr-TCPP was named Zr-TCPP-RFx, where x represents the carbon number of the perfluorinated group (CxF2x+1COOH). Longer alkyl chains of the perfluorocarboxylates used to prepare Zr-TCPP-RFx led to greater hydrophobicity. Photocatalytic H2O2 production was promoted by the modification of Zr-TCPP with perfluorocarboxylates. The length of the perfluoroalkyl chain plays a critical role in the enhancement of photocatalytic H2O2 production, and optimization of the chain length resulted in a 7.2-fold increase in activity compared with that of the pristine hydrophilic Zr-TCPP. Perfluoroalkyl-functionalization improves the hydrophobicity of the MOF, leading to suppression of H2O2 decomposition. The optimized hydrophobicity facilitates O2 enrichment at the photocatalyst surface and enhances the selectivity of the two-electron water oxidation pathway, thereby improving photocatalytic H2O2 production. [1] Y. Kondo, S. Mizutani, Y. Kuwahara, K. Mori, T. Sekino, T. Zhang, Z. Bian, H. Li, H. Yamashita, Chem. Eur. J., 2026, 32, e00026. [2] Y. Kondo, Y. Kuwahara, K. Mori, H. Yamashita, Chem, 2022, 8, 2924-2934. [3] Y. Zhao, Y. Kondo, Y. Kuwahara, K. Mori, H. Yamashita, Appl. Catal. B: Environ., 2024, 351, 123945. [4] Y. Kondo, K. Honda, Y. Kuwahara, K. Mori, H. Kobayashi, H. Yamashita, ACS Catal., 2022, 12, 14825-14835. [5] Y. Kondo, K. Hino, Y. Kuwahara, K. Mori, H. Yamashita, J. Mater. Chem. A, 2023, 11, 9530-9537. [6] Y. Zhao, H. Ge, Y. Kondo, Z. Guo, Y. Kuwahara, K. Mori, T. Sekino, Z. Bian, H. Yamashita, ACS Catal., 2025, 15, 11313-11325.[7] Y. Kondo, K. Honda, S. Mizutani, Y. Kuwahara, K. Mori, T. Sekino, H. Yamashita, Appl. Catal. B: Environ., 2026, 391, 126632.[8] Y. Kondo, S. Mizutani, Y. Kuwahara, K. Mori, T. Sekino, H. Yamashita, J. Mater. Chem. A, 2025, 13, 3701-3710.

Graphene coating of Zn Metal Powder for Aqueous Zn-ion Batteries

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Aqueous zinc metal batteries (AZMBs) are promising for safe, high-energy storage, with zinc powder offering greater design flexibility over traditional zinc foil. However, zinc powder's surface instability, causing side reactions and dendrite formation, limits its use. To address this, we developed a graphene-coated zinc powder anode (Gr_Zn) using a mechanofusion dry-coating technique. This method ensures uniform graphene coverage, stabilizing the electrode-electrolyte interface and suppressing parasitic reactions. The hydrophobic graphene layer alters electrolyte solvation, promoting uniform zinc deposition. This approach provides a practical solution for advancing AZMBs with zinc powder anodes, enhancing their performance and stability. The resulting graphene-coated Zn powder (Gr_Zn) exhibits stable cycling with a low voltage hysteresis of 16.1 mV over 640 h at 1 mA cm−2, outperforming zinc foil and bare Zn powder electrodes. Moreover, Gr_Zn delivers high-rate capability and exceptional high areal capacity (>20 mAh cm−2) in full-cell and pouch-cell configuration [1]. [1] Advanced Science, e77287, https://doi.org/10.1002/advs.77287

Partially Thiolated, Atomically Precise Gold Clusters as Model Heterogeneous Catalysts

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The discovery of unprecedented catalytic properties of nano-sized gold for CO oxidation[1] stimulated researchers to elucidate the origin of size-specific catalytic properties; thereby, it has been a central interest in nanoscience. However, technical challenges in synthesizing size-controlled gold nanoparticles on solid support, especially in the cluster-size regime (typically ≤2 nm) with atomic precision, have hindered in-depth investigation. Recent advances in nanotechnology have enabled the synthesis of ligand-protected gold clusters with atomic precision over the past two decades. Thus, we addressed this synthetic challenge through the thermal removal of ligands from atomically precise, ligand-protected gold clusters on a solid support.[1,2] Although this approach enabled us to create Au cluster catalysts with atomic precision, the resulting clusters often lose their size accuracy during catalysis, which hinders the study of size effects. Therefore, we must suppress the diffusion of the Au clusters on the support to overcome this inherent problem. Recently, we have developed a new approach to suppress aggregation using non-bonding interactions, such as van der Waals or electrostatic interactions, between the organic ligands and supports. [3-7] This method intentionally leaves the ligands between the cluster and support through multiple ligand-support interactions under thermal treatment while removing other ligands exposed to the surface, which forms catalytically active exposed gold sites. The resulting partially ligated Aun clusters balance both high catalytic activity and durability during catalysis. First, we evaluated the importance of the remaining ligands on durability by comparing the benzyl alcohol oxidation activity at 80 °C over partially thiolated or bare

Au25 cluster catalysts. The partially thiolated catalyst exhibits a similar initial activity to the bare catalyst and maintains the activity for complete conversion, whereas the bare catalyst was deactivated at the initial stage.[3] These results clearly represent the importance of our strategy for balancing the activity, durability, and accuracy in size. Based on the platform, we investigated the effect of the ligand, support, and cluster size on the catalytic properties by modifying these parameters. In addition, we have recently succeeded in the synthesis of the ligand- protected, atomically precise gold clusters in a wide size range by solubility-mediated growth control during the synthesis.[8] Now, we further broaden the variety of catalysts and investigate the catalytic properties of these unique materials. We will introduce some of the examples in the presentation. References:

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Development of Organic Energy Materials

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Toward the realization of a sustainable society, the development of innovative organic energy materials, which are composed of earth-abundant elements and which play a role in energy conversion and storage, is highly required. In this lecture, I will describe several examples of organic energy materials (organic polymeric materials) with the following energy-related functions (1)—(5). (1) Charge storage and transport. (2) Proton storage and transport. (3) Hydrogen gas production and storage. (4) gas selective adsorption and storage. (5) Photocatalysis and clean energy production. The latest efforts towards creation of highly durable organic materials via deuteration will be also introduced. In addition, this presentation will also cover the prototyping of applications or devices using these organic energy materials. For example, ① Organic secondary batteries which are composed of organic electrode-active materials. ② Compact fuel cells which use organic electrode-active materials as an anode. ③ Hydrogen carrier materials (Polymeric hydrogen storage materials) which chemically fix and release hydrogen gas (H2) even under mild conditions. ④ CO2 storage material. ⑤ On-site clean energy (e.g., H2 and H2O2) production which uses organic energy materials as a photo(electro)catalyst or electrocatalyst.

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Particle-Selective Consolidation with a Citrate-Crosslinked β-Cyclodextrin Co-Binder for Dry-Processed Thick Cathodes

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Solvent-free dry processing offers a route to high-loading lithium-ion battery cathodes, but compaction during polytetrafluoroethylene (PTFE) fibrillation can fracture Ni-rich secondary particles. Controlling which particles are consolidated, and the size of the resulting aggregates, may help manage these mechanical stresses. Here, we investigate a citrate-crosslinked β-cyclodextrin co-binder (BCC) for selective consolidation of the small-particle fraction in dry-processed thick cathodes. Granular discrete element method (DEM) simulations were used to examine how selective particle consolidation changes contact forces. Consolidating only small particles into aggregates approximately equal in diameter to the large particles reduced the simulated peak contact force on the large particles by approximately 24%. This result provided a particle-size criterion for the co-binder design. Size- resolved X-ray photoelectron spectroscopy (XPS) confirmed preferential BCC coverage of the small-particle fraction. Electrodes were prepared with a total binder content of 2.2 wt%, with BCC replacing 25% of the binder. At an areal capacity of 10 mAh cm^{-2}, this formulation exhibited the lowest tortuosity (1.23) and the most uniform adhesion among the formulations compared, while retaining 87% of its capacity after 100 cycles. These results support particle-selective consolidation as a design approach for controlling granule architecture in dry-processed thick cathodes and identify BCC as a co-binder for implementing this approach.

Session: Biomaterials, Bioengineering and Bio-related Applications

The Importance of Assessing the Health Impact of Graphenic Carbon Materials

Alberto Bianco, Université de Strasbourg, France

Next-Generation Polymeric Materials Development and Their Clinical Applications

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In this talk, the speaker will discuss next-generation polymeric material development and their clinical applications,particularly siloxane-based polymers. Siloxane-based polymers have emerged as highly promising materials forbiomedical applications owing to their structural flexibility, biocompatibility, and tunable physicochemicalproperties. A comprehensive overview of recent advances in the design, synthesis, and translational potential ofsiloxane-based polymers tailored for transdermal and targeted drug delivery systems is discussed [Ref: 1-5]. Keyhighlights include the development of acid-initiated ring-opening polymerization platforms, such as PDDS and T2polymers, which exhibit controllable viscosity, degradability, and encapsulation efficiency. Among these, the C2polymer (PDDS series) demonstrated superior biocompatibility, balanced hydrophilicity, and in vivo performance inmelanoma therapy models, achieving deep skin permeation and enhanced anticancer efficacy. In parallel, 5-AP, a 5-aminolevulinic acid-conjugated siloxane hybrid, was introduced as a novel photodynamic therapy (PDT) agent. Thismaterial enabled the transdermal delivery of 5-ALA and in situ generation of protoporphyrin IX (PpIX), leading toselective ROS-mediated tumor destruction upon light activation. Furthermore, CPMD- and DNZ-loaded T2polymers exemplify the versatility of siloxane frameworks for fat reduction and neurodegenerative therapy,respectively, demonstrating controlled release, skin permeation, and therapeutic efficacy with minimal toxicity.Together, these studies suggest that siloxane-based polymers can be systematically engineered as multifunctionaltherapeutic platforms for next-generation transdermal biomedical applications.References

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Biopolymer Piezoelectric Technology for Health Applications

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Flexible electronics for health monitoring require materials and devices with unique properties such asbiocompatibility, flexibility, high sensitivity, and body compliance. Skin and wearable sensors enable the detection ofpathophysiological biomechanical signals and symptoms of disorders and diseases in an unobtrusive manner. In recentyears, compliant and flexible piezoelectric thin-film materials have enabled the demonstration of piezoelectric skin-compliant biointerfaces for stimulating, sensing, and monitoring biomechanical signals, and for harvesting energy forautonomous microsystems in medical devices. The most recent generation of flexible piezoelectric biocompatible thinfilms materials includes lead-free inorganic piezoelectrics on polymeric substrates, synthetic polymers andbiopolymers. The current challenge relies on producing efficient flexible piezoelectric materials to be safely appliedto the human body and processed in functional devices for in-vivo experiments.In this presentation, the material and device technology of chitosan-based piezoelectric biopolymers will be discussed[1]. This material system will be shown to combine good mechanical and piezoelectric properties, safety, andbiocompatibility. Despite not requiring poling (a critical process for aligning individual dipole moments), recordpiezoelectric coefficients have been achieved in chitosan and chitin thin films. The dispersion of cellulose nanocrystalsand drug molecules in chitosan films, the direct electrodeposition of chitosan films on conductive substrates and themicropatterning of its surface to induce flexoelectric properties are currently opening the route towards ultra-efficientsustainable piezoelectric sensors and actuators for healthcare applications [2,3].References[1] G. de Marzo, V.M. Mastronardi, L. Algieri, F. Vergari, F. Pisano, L. Fachechi, S. Marras, L. Natta,Spagnolo,V. Brunetti, F. Rizzi, F. Pisanello, and M. De Vittorio, “Sustainable, Flexible, and Biocompatible EnhancedPiezoelectric Chitosan Thin Film for Compliant Piezosensors for Human Health,” Adv. Electron. Mater. 9(9),2200069 (2023).[2] Antonaci, V., de Marzo, G., Blasi, L., Brunetti, V., Binetti, E., Fachechi, L., Marras, S., Qualtieri, A., Rizzi, F., &de Vittorio, M. (2026). Biodegradable chitosan-cellulose and sub-spherical nanocrystals composite piezoelectrithin film. Npj Flexible Electronics, 10(1), 55.[3] Gaia de Marzo, Valentina Antonaci, Virgilio Brunetti, Laura Blasi, Luca Fachechi, Sergio Marras, AntonioQualtieri, Francesco Rizzi, Roberto Fiammengo, and Massimo De Vittorio, Tailored piezoelectric chitosan thinfilm for ultrasound-controlled drug delivery, Nature Communications Materials 7, 174 (2026).

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Diamond-Like Carbon Coating Modulates Staphylococcus aureus Biofilm Formation on Polymeric Medical Substrates Under Static and Flow Conditions

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Device-associated infections remain a major challenge in polymeric medical devices such as vascular grafts, catheters,drainage tubes, and extracorporeal circuits. Because bacterial adhesion to the inner surface of these devices can initiatebiofilm formation, surface engineering of polymeric biomaterials is an important strategy for reducing infection risk.Diamond-like carbon (DLC) coating has attracted attention as a chemically stable and biocompatible surfacemodification; however, its biological effects on polymeric substrates may not be determined solely by the presence ofthe coating. In particular, polymeric materials differ substantially in surface chemistry, flexibility, roughness, andwettability, and medical devices are often used under dynamic fluid conditions rather than static environments.Therefore, the anti-biofilm potential of DLC should be evaluated as a substrate- and environment-dependentbiointerface phenomenon.In this study, we investigated the effects of inner-lumen DLC coating on Staphylococcus aureus biofilm formation andbacterial adhesion using clinically relevant polymeric tube materials. Eight polymeric substrates, including silicone,polyethylene, polyurethane, expanded polytetrafluoroethylene, and several polyvinyl chloride-based tubes, wereexamined with or without DLC coating. The luminal surfaces were exposed to S. aureus for 24 hours under either staticculture conditions or perfusion using an in vitro flow circuit designed to reproduce fluid exposure to the inner surfaceof tubular medical devices. Biofilm formation was quantified by Crystal Violet staining, while surface-adherentbacteria were evaluated by scanning electron microscopy.The results demonstrated that biofilm formation and bacterial adhesion were strongly influenced by the type ofpolymeric substrate and by the contact condition. Flow exposure generally enhanced both biofilm formation andbacterial adhesion compared with static culture, indicating that hydrodynamic conditions can substantially modifybacterial behavior on polymeric device surfaces. In contrast, DLC coating alone did not produce a uniform anti-biofilmeffect across all substrates. DLC reduced biofilm formation on selected polymeric materials, whereas its effect waslimited or absent on others. Moreover, DLC did not consistently reduce the number of adherent bacteria, suggestingthat suppression of total biofilm biomass and suppression of initial or residual bacterial colonization are not equivalentoutcomes. The weak relationship between Crystal Violet-based biofilm biomass and SEM-based bacterial countsfurther supports the concept that biofilm development reflects multiple processes, including bacterial attachment,extracellular matrix production, and biofilm maturation.These findings suggest that pure DLC should not be regarded simply as a universally antibacterial coating. Rather,DLC functions as a context-dependent biointerface-

modifying layer whose effects are governed by the underlyingpolymeric substrate and the fluid environment. This study highlights the importance of evaluating surface-modifiedpolymeric medical devices under clinically relevant flow conditions and provides a materials-based framework fordesigning infection-resistant biointerfaces for tubular medical devices.Keywords: Diamond-like carbon; Biofilm formation; Staphylococcus aureus; Polymeric medical devices; Flow condition

Biomaterials from Extreme Environments: The Promise of Microbial Biopolymers

Sandra Pucciarellia*, Maria Chiara Biondinia

Microorganisms thriving in extreme environments have evolved unique adaptive strategies, including the production of biomaterials as a response to environmental stressors (1). With the global demand for sustainable and high-performance biomaterials on the rise, these microbial products represent a promising frontier in material science. Microbial biomaterials stand out for their exceptional properties, such as high purity, mechanical strength, andbiocompatibility. Microorganisms from Antarctica offer a particularly untapped resource for discovering novelbiopolymers with unique structural and functional characteristics. Among emerging biomaterials, bacterial cellulose(BC) is generating significant interest due to its unique characteristics. Unlike traditional plant-based materials, BCcan be produced through eco-friendly processes, making them ideal for a wide range of applications. In this study,marine bacterial strains isolated from a consortium associated with the Antarctic ciliate Euplotes focardii were testedfor cellulose production. We found that these Antarctic strains can produce BC in conditions that appear unique, andthe final BC product is structurally different from that obtained from the well-known BC producer Komagataeibacterxylinus. The produced BC possesses different morphology, according to the protocol used: in HS medium, theproduced BC appears as a sheet-like product, whereas in medium containing either yeast extract or nutrient broth andsea water under shaking conditions, the product appears as spherical flocculates. X-ray diffraction patterns of dispersedand spherical bacterial cellulose produced by the strain named Pseudomonas sp. ef1 in static and shaking conditions,showed that the former corresponds to type I cellulose, whereas the latter to type II (2). The formation of cellulose IImediated by bacteria under agitation may be attributed to localized thermal effects induced by mechanical stirring.Furthermore, we found that the type I Pseudomonas sp ef1 cellulose impart unique functional properties to materiallike paper, including water and oil resistance. The versatility of microbial biopolymers opens innovative applicationsacross multiple industries, including biomedicine, food packaging, pharmaceuticals, and environmental technologies.By harnessing the potential of these microorganisms, researchers can develop sustainable, high-performance materialsthat address current challenges in material science and contribute to a greener, more circular economy.1- Ramasamy KP, Mahawar L, Rajasabapathy R, Rajeshwari K, Miceli C and Pucciarelli S (2023) Comprehensiveinsights on environmental adaptation strategies in Antarctic bacteria and biotechnological applications of cold adaptedmolecules. Front. Microbiol. 14:1197797. doi: 10.3389/fmicb.2023.11977972- Biondini, M.C.; Di Sessa, M.; Vassallo, A.; Chiappori, F.; Zannotti, M.; Mancini, A.; Giovannetti, R.; Pucciarelli,S. Cellulose and Cellulose Synthase in a Marine Pseudomonas Strain from Antarctica: Characterization, AdaptiveImplications, and Biotechnological Potential. Mar. Drugs 2025, 23, 410. https://doi.org/10.3390/md23100410

Next-Generation Molecularly Templated MaterialsFrom Biomimetics to Biosuperiors

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Biomimetic recognition utilizing molecularly imprinted polymers (MIPs) has proven itspotential by providing synthetic receptors for numerous analytical applicationsincluding liquid chromatography, solid phase extraction, biomimetic assays, andsensor systems. The inherent advantages of synthetic receptors and functionalizedmembranes in contrast to biochemical/biological recognition and immobilizationschemes include their robustness, synthetic versatility, and potentially lower costs. Inprinciple, molecularly imprinted/templated materials are an ideal molecular capturingmatrix tailorable for selective recognition or immobilization of a wide range ofmolecules, and even of entire organisms.Of particular interest is the development of biosuperior recognition schemes forselectively binding proteins and large biomolecules, as well as for controlled molecularrelease. While materials with recognition capabilities even for larger biomoleculeshave achieved substantial advancements, the synthesis of molecularly templatedmaterials with virus recognition properties remains challenging. We will discussinnovative strategies for developing biomimetic virus capture materials yieldingunprecedented selectivity. Finally, breakthrough approaches will be highlighted on 3printing of MIPs and simulation concepts for the first time providing strategies forgenerating 'virtually imprinted polymers' (VIPs).References[1,2] S. Zink et al, PCCP 20, 13145 (2018) & PCCP 20, 13153 (2018)[3,4] M. Gast et al, Anal. Chem. 90, 5576 (2018) & Anal. Chem. 92, 3050-3057 (2020)[5,6] S. Rajpal et al, J. Mater. Chem. B 10, 6618 (2022) & Scientific Reports 14, 23057 (2024)[7,8] B. Keitel et al, ACS App. Poly. Mat, 6, 3690 (2024) & Adv. Mat. Techn. 8, 2570003 (2025)

Label-free and Image-based Electrical Characterization of Cell Membrane

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The electrical properties of the plasma membrane reflect cell composition, morphology, and physiological state and therefore provide label-free markers for cell characterization. Electrorotation (ROT) can estimate membranepermittivity and cytoplasmic conductivity from frequency-dependent rotation of single cells exposed to a rotatingelectric field. However, conventional ROT measurements require cells to be individually trapped and replaced,limiting throughput and making population-level analysis difficult. Here, we present continuous-flow electrorotation(cROT) as a microfluidic approach for rapid evaluation of cell membrane electrical properties. The electrical torquearises from the phase difference between the applied field and induced cellular dipole and depends on the imaginarycomponent of the Clausius-Mossotti factor. Because this factor varies with excitation frequency, the rotationspectrum encodes information on membrane polarization and intracellular conduction. Population measurementsresolve variability associated with cell cycle, phenotype, stress, and chemical exposure. A higher-throughput ROTformat is required to capture cell-to-cell variability while retaining dielectric information. The cROT device consistsof a microchannel sandwiched between upper and lower substrates carrying interdigitated electrodes. Four phase-shifted alternating-current signals generate a rotating electric field in the cross-sectional plane of the channel, while dielectrophoretic forces position flowing cells within the measurement region. This configuration induces vertical cell rotation during translational motion and permits multiple cells to be analyzed successively without repeated manual trapping. Cell trajectories and angular velocities are extracted from time-resolved microscopy at multiple field frequencies. The rotational velocity can be measured by image analysis. The measured electrorotation spectra are then fitted with a single-shell dielectric model to determine membrane permittivity and cytoplasmic conductivity at the single-cell level.

Experimental results demonstrate that cROT combines the quantitative capability of electrorotation with the throughput and automation potential of microfluidics. The approach is noninvasive, label-free, and compatible with measurements of large cell populations, making it suitable for detecting changes in membrane composition, permeability, and physiological condition. The proposed method therefore offers a scalable route toward functional single-cell analysis.

Molecular Design of Porphyrin-Containing Glycopolymers for Biomedical Applications

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Since many synthetic photosensitizers, including porphyrin derivatives, exhibit poor water solubility, their biological availability and therapeutic efficacy are often limited. To address this issue, we designed a system combining porphyrins and carbohydrates using polymer chemistry. Water-soluble porphyrins and glycoporphyrins have been reported as hydrophilic compounds by other research groups, along with their successful applications in photodynamic therapy (PDT). Copolymerization afforded water-soluble glycopolymers capable of incorporating hydrophobic porphyrin units in aqueous media. Herein, we report the synthesis of porphyrin and N-acetyl-D- glucosamine (GlcNAc)-containing monomers and their copolymerization with acrylamide (AAm). Furthermore, the biological responses of the resulting glycopolymers containing porphyrin moieties toward cancer cells are evaluated. The water-soluble glycopolymers bearing porphyrin moieties exhibited biological activity against HeLa cells. Keywords: Carbohydrates, Glycopolymers, Polymerizations, Porphyrins, PDTReferences1) Y. Ishimaru, et al., ACS Omega 2023, 8, pp. 37329-37340.2) Y. Komano, et al., Biomacromolecules 2025, 26, pp. 3021-3031.

Molecular Engineering Enables Bright, Narrow-Emissive Carbon Dots for Multiplexed Super-Resolution Mapping of Organelle Dynamics

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Cells contain various organelles with different functions. Accurate differentiation and imaging of theseorganelle structures are prerequisites for accurately interpreting their physiological functions. Multicolorsimultaneous super-resolution imaging is an important method for capturing the dynamic synergy between differentorganelles, but it places extremely high demands on probe performance: it must simultaneously possess highbrightness, high photostability, high spectral resolution, good biocompatibility, and small size. Carbon dots haveadvantages such as resistance to photobleaching, high biocompatibility, and ultra-small size (2-5 nm), making themideal subcellular imaging probes. However, carbon dots prepared by traditional methods suffer from low quantumyield and limited multicolor emission, restricting their application in multicolor simultaneous super-resolutioimaging of organelles.To address these challenges, we systematically analyzed the core scientific question of "surface state-dominated luminescence," introducing multidimensional characterization techniques such as ultrafast transientabsorption spectroscopy, time-resolved emission spectroscopy, and nuclear magnetic resonance spectroscopy. Forthe first time, we elucidated the key regulatory roles of hydrogen bonding and polarization effects on the radiativetransitions of carbon dot surface states. Based on this, we proposed a molecularly engineered surface state regulationstrategy to achieve precise enhancement of the key performance characteristics of carbon dots. First, a synergisticregulation method of hydrogen bond elimination and polarization enhancement was established to suppress the nonradiative decay of carbon dot surface states and promote charge transfer, increasing the fluorescence quantum yieldof carbon dots from approximately 30% to a maximum of 98%, resulting in high-brightness functionalized carbondots. Second, a synergistic regulation method of dipole moment enhancement and conjugation extension wasestablished to reconstruct the surface charge distribution and energy level structure of carbon dots, extending theemission window from blue light (~450 nm) to red light (~950 nm) and compressing the full width at half maximum(FWHM) from approximately 150 nm to 65-90 nm, constructing a narrow-peak, tunable emission carbon dot probesystem.Using the newly created series of high-performance probes, high-density labeling and long-term continuoussuper-resolution imaging (up to 352 frames) of seven organelles in living cells-mitochondria, endoplasmicreticulum, lysosomes, microtubules, nucleus, lipid droplets, and cell membrane-were achieved. For the first timehigh-frequency interaction events (18-23 times/second) between four organelles under acute hypoxia conditionswere captured, revealing the spatiotemporal adaptation mechanism of organelle interaction networks.References：[1] Y. Chen, Z. Liu, Y. Wang, Y. Mei, J. Sun, X. He, J. Wan, Y. Tian, Nat. Chem. Biol. 2026, DOI:10.1038/s41589-026-02158-5.[2] Z. Liu, J. Li, C. Zhao, Z. Zhang, P. Wu, J. Chen, X. He, S. Zhang, Y Tian, Adv. Mater. 2025, 37, 2410786[3] Y. Zhao, Y. Mei, J. Sun, Y. Tian, J. Am. Chem. Soc. 2025, 147, 5025.[4] Y. Zhao, Y. Mei, Z. Liu, J. Sun, Y. Tian. Nat. Commun. 2025, 16, 1848.[5] B. Kong, A. Zhu, C. Ding, X. Zhao, B. Li, Y. Tian, Adv. Mater. 2012, 24, 5844.[6] A. Zhu, Q. Qu, X. Shao, B. Kong, Y. Tian, Angew. Chem. Int. Ed. 2012, 51, 7185.

Giant Piezoresponse in Nanoporous (Ba,Ca)(Ti,Zr)O3 Thin Films Enabled by Pore-Induced Lattice Strain

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Lead-free piezoelectric materials with high electromechanical performance are strongly desired for next-generation sensors, actuators, and energy-harvesting devices. Although Pb(Zr,Ti)O3 (PZT) and related Pb-basedmaterials exhibit excellent piezoelectric properties, their toxicity has driven intensive efforts to developenvironmentally sustainable alternatives [1]. Among them, Ca/Zr co-doped BaTiO3, (Ba,Ca)(Ti,Zr)O3 (BCZT), is apromising candidate because of its enhanced piezoelectricity near the morphotropic or polymorphic phase boundary[2]. Beyond conventional composition and crystal-structure engineering, nanoscale morphology offers another routeto control ferroelectric properties through local strain [3,4]. Here, we demonstrate that a nanoporous architectureinduces exceptionally large lattice strain and a giant piezoresponse in lead-free (Ba0.85Ca0.15)(Ti0.9Zr0.1)O3 thin films.Nanoporous BCZT films were fabricated by a sol–gel-based soft-templating method using polystyrene-block-poly(ethylene oxide) (PS-b-PEO) as a pore-directing agent. After calcination at 650 °C, elongated nanoporessurrounded by highly crystallized BCZT frameworks were obtained. X-ray diffraction confirmed the perovskitephase, while annular dark-field scanning transmission electron microscopy and elemental mapping verified theincorporation of Ca and Zr into the BaTiO3 lattice.The effect of the nanoporous structure on local lattice deformation was investigated by high-resolutionscanning transmission electron microscopy combined with geometric phase analysis. The local strain in thenanoporous BCZT film exceeded approximately 30%, whereas that of the nonporous BCZT film was approximatel0.3%. Thus, pore formation produced a nearly two-order-of-magnitude enhancement in local strain, demonstratingthat the pore-wall geometry generates intense lattice distortion. The observed correspondence between the enlargestrain field and the enhanced piezoresponse indicates that nanoscale pore-induced deformation is a key factorgoverning the electromechanical response.Piezoresponse force microscopy further revealed a remarkable enhancement in electromechanical responseThe nanoporous BCZT film exhibited a remanent d33 of approximately 7500 pm V−1, more than ten times larger thanthe approximately 550–600 pm V−1 obtained for the nonporous film. Clear 180° phase switching and d33–voltagehysteresis behavior were also observed. In addition, the nanoporous film exhibited a dielectric constant oapproximately 1500, compared with approximately 1000 for the nonporous film, while maintaining relatively lowdielectric loss and adequately low leakage current density.The enhanced piezoresponse is attributed to pore-induced anisotropic stress and the associated distortion ofthe BCZT lattice, which promote polarization and electromechanical deformation. Importantly, the enhancemenwas achieved simply by introducing nanoscale porosity without constructing more complicated nanowire, nanofiber,or core-shell architectures. These results demonstrate that nanoscale morphology and pore-derived strain can serveas effective materials-design parameters, complementing conventional composition- and crystal-structure-basedapproaches. Nanoporous BCZT therefore provides a simple strategy for developing high-performance lead-freepiezoelectric thin films for sensing, actuation, dielectric capacitors, and high-density energy-harvesting applications.References[1] K. Uchino, Advanced Piezoelectric Materials, 2nd ed., Woodhead Publishing, 2017.[2] W. Liu and X. Ren, Phys. Rev. Lett. 103, 257602 (2009).[3] N. Suzuki et al., Chem. Eur. J. 20, 11283–11286 (2014).[4] N. Suzuki et al., APL Mater. 5, 076111 (2017).

Photoinactivation of S. aureus by molybdenum cluster and graphene oxide coatings

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To respond to the growing issue of microbial resistance, this research investigates antimicrobial coatings that usevisible light to inactivate bacteria, a process known as photodynamic inactivation.This thesis is supported by the University of Rennes and the Laboratory for Innovative Key Materials and Structures(LINK), that are part of the EIG Concert Japan PHOTOMOS-H 2 O project. It involves collaboration with the IIC(Czech Republic), Waseda University (Japan), the University of Orléans (France), and CNRS (France). The aim ito develop innovative hybrid coating films that can effectively prevent bacterial growth.The approach focuses on integrating light-activated singlet oxygen 1 O 2 (1 Δ g) generators, octahedral molybdenucluster complexes [Mo 6 I 8 (N 3) 6] 2- (Mo 6) [1-2] onto graphene oxide (GO) and reduced graphene oxide matrices (rGO)[3].To create thin layers incorporating these components, two distinct techniques are employed: electrophoreticdeposition and dip-coating. Initial results with molybdenum clusters are promising, as bacterial inhibition rates foS. aureus drop below 2%. However, these rates remain inconsistent when Mo 6 is combined with GO or rGO,possibly due to interactions between them. Furthermore, singlet oxygen is undetectable upon irradiation of these thinfilms, suggesting that an alternative mechanism, such as other reactive oxygen species like hydroxyl radicals, maybe responsible for the observed antibacterial effects.Additionally, another project has recently begun in collaboration with the National Institute for Materials Scienc(NIMS) in Japan. This project aims to incorporate Mo 6 compounds into porous anodised aluminium oxide. Thismaterial acts as an optical fibre, offering the advantage of light conduction, which is expected to enhance thactivation of the clusters. Furthermore, these surfaces should exhibit greater mechanical resistance compared tMo 6 @GO or Mo 6 @rGO.Hybrid films are analysed by SEM, EDS, XPS, and photoluminescence measurements. Singlet oxygen ismeasuring thanks spectroscopy and its emission is at 1270 nmThis study demonstrates the potential of these hybrid coatings as an alternative solution to combat bacterialinfections, especially in the context of increasing antibiotic resistance.

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An evaluation method for lipid membrane viscosity via the diffusion of particles adsorbed on lipid membranes

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Biological membranes composed of lipid bilayers perform various essential functions, including protein-mediatedmaterial transport, signal transduction, and cell division. Membrane viscosity governs the lateral transport of lipidsand proteins, the movement of membrane domains, and overall cell membrane fluidity. Therefore, evaluatingmembrane viscosity is crucial for clarifying these biological functions. Most previous studies have assessed membraneviscosities using fluorescent probes[1]; however, such molecular-scale probes cannot determine the viscosity involvedin domain flow and overall membrane flow because such probes strongly reflect the local, molecular-scaleenvironment within membranes. Recently, a macroscopic viscosity measurement approach by considering the fluiditof the entire cell membranes has been proposed[2]. Nevertheless, a quantitative approach for evaluating membraneviscosity at the submicron scale has not been established, although the viscosities experienced by nano–submicronsized objects (e.g., lipid rafts) are likely to be the key for the dynamics and functions of biological membranes.In this study, we proposed a novel viscosity evaluation method based on the diffusion behavior of submicron-sizedcolloidal particles. It has been reported that positively charged poly(N-isopropylacrylamide) (PNIPAM) particles areable to adsorb and diffuse on lipid membranes[3]; thus, we prepared positively charged, green-fluorescent PNIPAparticles (840 nm in diameter) as probes for the viscosity measurement. Giant Unilamellar Vesicles (GUVs) wereprepared as model lipid membranes, which were composed of 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC),cholesterol, and a red-fluorescent lipid in specified proportions. Using confocal laser microscopy, we tracked thdiffusive motions of single PNIPAM particles adsorbed on GUVs, and diffusion coefficients of particles werecalculated from the trajectories. To estimate the quantitative relationship between diffusion coefficients of particlesand membrane viscosities in the above particle-adsorbed GUV system, numerical simulations based on the finiteelement method were performed. The stress acting on the particle surface with a constant velocity boundary conditionwas calculated with membrane viscosity as parameter. The diffusion coefficient was obtained from the calculatedstress via the Einstein diffusion-mobility equation. By comparing the experimentally measured diffusion coefficientswith the calculated diffusion coefficients-viscosity relationship, membrane viscosities of GUVs prepared in this studywere estimated. The estimated viscosities were close to those reported in previous studies, suggesting that the proposedapproach in this study is viable. The proposed approach evaluating the “submicron scale membrane viscosity” can bea novel tool for elucidating the functions of biological membranesReferences:[1] A. S. Kashirina et al., Scientific Reports, 10, 14063, 2020.[2] Y. Sakuma et al., Biophysical Journal, 124 (19), 3304–3318, 2025.[3] M. Wang et al., Proc. Natl. Acad. Sci. U.S.A., 116 (12), 5442–5450, 2019.

Iron-Based Layered Double Hydroxide Nanoparticles Co-Loaded with S- Nitrosoglutathione: A Multifunctional Sonosensitiser Platform with Tunable ROS

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Introduction. Layered double hydroxides (LDHs) are two-dimensional anionic clays whose tunablecomposition, high anion-exchange capacity, and pH-responsive dissolution make them attractiveinorganic scaffolds for stimuli-responsive nanomedicine. Incorporating redox-active transition metals intothe LDH lattice offers a route to sonosensitive materials that generate reactive oxygen species (ROS)under ultrasound and provide intrinsic magnetic resonance imaging (MRI) contrast. Here, we report thdesign of an iron-based LDH co-loaded with S-nitrosoglutathione (GSNO), Fe-LDH@GSNO, whichintegrates ultrasound-triggered ROS generation, nitric oxide (NO) release, and T2-weighted MRI contrastwithin a single inorganic host.Materials and Methods. Fe-LDH nanoparticles were synthesised and subsequently loaded with GSNvia anion exchange. GSNO loading was quantified by UV-Vis spectroscopy (λ335, R^2 = 0.9924) acrossFe-LDH concentrations of 0.24–2.38 mg/mL. Ultrasound-triggered (50 kHz, 2 W/cm^2) generation ofhydroxyl radical (•OH), superoxide anion ($O_2•^-$), and singlet oxygen ($^1O_2$) was probed using CCA,DHE, and DPBF, respectively, in an H_2O_2-mimicked tumour microenvironment to assess redox-dependent activity. NO release under ultrasound was monitored for over 10 minutes. T1 and T2 relaxivitywere characterised to evaluate MRI contrast behaviour. Biological compatibility and selectivity werescreened in CT26 colorectal cancer cells and 3T3 normal fibroblastsResults and Discussion. The Fe-LDH host supported efficient, ultrasound-triggered generation of •OH,$O_2•^-$, and $^1O_2$, with ROS output enhanced in the H_2O_2-rich environment, indicating that the irocentres couple sonodynamic activation with Fenton-type redox chemistry characteristic of the tumourmicroenvironment. GSNO co-loading conferred controllable NO release, sustained over 10 minutes ofstimulation, without compromising the sonosensitising function of the host. Relaxivity characterisationconfirmed the material functions as a T2-weighted contrast agent, establishing the iron lattice as a dualpurpose structural and imaging element rather than a passive carrier. In cellular studies, the combinedmaterial-plus-ultrasound treatment produced selective elevation of ROS and reduced viability in CT26cells, while sparing 3T3 fibroblasts, demonstrating that the material's activity is contingent on bothultrasound and the target microenvironment.Conclusion. Fe-LDH@GSNO demonstrates how a single inorganic 2D host can be engineered to unitesonodynamic ROS generation, gasotransmitter delivery, and MRI contrast. The design highlights redox-active LDHs as a versatile materials platform for stimuli-responsive theranostics and warrants furtherinvestigation of composition–function relationships.

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Mesoporous Gold SERS Platform for Extracellular Vesicle-based Detection of Ovarian Cancer

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Early detection of ovarian cancer (OC) is critical for improving patient outcomes, with >90% survivalwhen diagnosed at stages I–II, compared with only 20–40% at stages III–IV. This highlights the urgentneed for sensitive and minimally invasive approaches capable of detecting OC at an early stage. Tumor-derived extracellular vesicles (EVs) are particularly promising biomarkers because they circulate iaccessible biofluids and carry molecular information from their cells of origin. To harness this diagnosticpotential, we developed a mesoporous gold-based biosensing platform that combines single-antibody EVcapture with surface-enhanced Raman spectroscopy (SERS) for sensitive and quantitative detection ofcirculating EVs in patients with OC. To identify the most informative EV targets for this platform, wefirst applied machine learning and computational analyses to three OC and healthy-control datasetsidentifying four promising surface biomarkers: CLDN3, FOLR1, CD24, and VTCN1. As an initial singlebiomarker validation, mesoporous gold substrates functionalized with 4-MBA and anti-CD9 were used tocapture EVs, while Claudin-3-targeted DTNB SERS nanotags provided signal amplification. Using SKOV-3-derived EVs (10 2 -10 9 EVs/mL), the platform showed a strong concentration-dependent response (R = 0.97) and an ultrasensitive detection limit of 80 EVs/mL. Importantly, while CA-125 achieved anAUROC of 0.96 with 90% sensitivity and 95% specificity, the SERS platform correctly classified allevaluated patients, achieving an AUROC of 1.00 with 100% sensitivity and specificity. Building on thisproof-of-concept, the remaining biomarkers will be integrated into a multiplex platform to furtherstrengthen early OC detection. Overall, this rapid, ultrasensitive EV liquid-biopsy strategy offers promising pathway toward detecting OC in asymptomatic women and enabling earlier, personalizedintervention.

Session: Electronics and Optical Materials

Van der Waals assembly of 2D materials for reconfigurable electronics

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Two-dimensional (2D) nanomaterials have emerged as promising building blocks for electronic applications, owingto their diverse and remarkable electrical properties. Over the past decade, solution-based processing—includingboth direct exfoliation and intercalation-based exfoliation—has been widely regarded as a viable route for the largescale production of 2D materials. However, the resulting morphology of the nanosheets is highly dependent on thprocessing method, which is a key factor in minimizing sheet-to-sheet contact resistance by enabling the formatioof high-quality van der Waals interfaces. In this talk, I will present our latest advances in the van der Waalsassembly of 2D materials for scalable electronic applications. Our approach utilizes a molecular intercalation-assisted electrochemical exfoliation technique to produce 2D materials with distinct electronic properties, includingmetals, semiconductors, and insulators. These materials can then be integrated into a range of electronic devices,such as transistors, diodes, logic gates, and photodetectors. Furthermore, our solution-based strategy enablesprinting-based device fabrication without the need for conventional patterning processes.

Development of Small-molecule and Polymeric Semiconductors for High-performance Organic Photodetectors

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Organic photodetectors (OPDs) have been actively studied because of their advantages, including light weight,tunable absorption range, and compatibility with large-area and high-resolution image sensors. In particular, organicsemiconductors can be molecularly designed to control their optical absorption, energy levels, intermolecularinteractions, and charge-transport properties. In addition, both solution processing and vacuum deposition can beused for OPD fabrication, depending on the molecular structure and target application. [1]Recently, we developed several polymeric and small-molecule semiconductors and investigated their photodetectionproperties in solution-processed andvacuum-deposited OPDs. For solution-processed OPDs, conjugated polymersemiconductors were designed by controlling the backbone structure and side-chain functionality. We found thatalkyl side-chain engineering is a particularly important synthetic factor that affects not only intermolecular orderingbut also dark-current suppression. Through careful control of the alkyl side chains, the specific detectivity could bimproved by more than two orders of magnitude. In addition, precise control of the π-spacer structure was found toplay an important role in optimizing electron transport and further improving OPD performance. [2, 3]For vacuum-deposited OPDs, we developed thermally stable small-molecule semiconductors with strong absorptionin the visible-to-near-infrared (NIR) region. Molecular conjugation, electron-withdrawing ability, and moleculardipole were systematically controlled to tune the absorption range, energy levels, molecular packing, and charge-transport properties of the

deposited films. In particular, these vacuum-depositable materials are highly suitable forvertically integrated device structures with conventional Si photodetectors and for the development of portable X-ray imaging sensors. The compatibility of vacuum deposition with existing semiconductor fabrication processes alsoprovides a clear advantage for practical device integration and suggests strong potential for future commercialapplications. [4, 5]References

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III–V Thermophotovoltaic Cells for Low-Cost Thermal Energy Conversion Systems

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Thermophotovoltaic (TPV) technology directly converts thermal radiation into electricity using photovoltaic cellsand has attracted considerable attention for waste heat recovery (WHR), thermal energy storage (TES) [1], anddistributed power generation [2]. III–V compound semiconductors have been extensively studied because of theirhigh radiative efficiency, tunable bandgaps [3], and compatibility with thin-film architectures incorporating back-surface reflectors (BSRs). Specifically, air/Au BSR TPV cells recycle sub-bandgap photons [4, 5], thereby reducingparasitic heat absorption and improving overall system efficiencyThe performance and economic feasibility of a TPV system strongly depend on the spectral matching of thermalemission to the cell bandgap, which influences the achievable efficiency and power density. For relatively lowsource temperatures of approximately 1000–1300 °C, low-bandgap materials such as InGaAs can be advantageousbecause they absorb a larger fraction of the available thermal radiation. At higher temperatures, however, practicallosses – including voltage loss, carrier recombination, series-resistance loss, and thermalization – becomeincreasingly important. Under these conditions, larger-bandgap III–V cells can offer higher output voltage andgreater tolerance to these losses, potentially achieving higher efficiency and power density. Thus, temperature-dependent bandgap optimization is essential for balancing TPV performance and system cost.

This talk presents the temperature-dependent optimization of III–V absorber bandgaps for TPV energy conversion.The analysis compares candidate III–V materials across a broad range of source temperatures while accounting forboth fundamental spectral considerations and practical cell-level losses. The resulting efficiency and power densitycharacteristics are then incorporated into techno-economic models of TPV systems designed for WHR and TEapplications. Particular attention is given to the trade-offs among source temperature, cell bandgap, cell performancesystem configuration, and cost. The results demonstrate that bandgap selection should be based not solely onmaximizing spectral absorption but on the combined optimization of device performance and system economics.This framework provides practical guidelines for selecting III–V materials and designing

cost-effective TPsystems for different thermal energy applications.AcknowledgemenThis research was supported by the Global-Learning & Academic Research Institution for Master's, Ph.D. studentsand Postdocs (LAMP) Program of the National Research Foundation of Korea (NRF), funded by the Ministry oEducation (No. RS-2024-00443714).Reference1. Datas, A., et al., Latent heat thermophotovoltaic batteries. Joule, 2022. 6(2): p. 418-443.2. Lim, J., Optimizing III-V thermophotovoltaic bandgaps for cost-effective thermal energy conversion.Energy Conversion and Management, 2026. 365: p. 121815.3. Roy-Layinde, B., et al., High-efficiency air-bridge thermophotovoltaic cells. Joule, 20244. Fan, D., et al., Near-perfect photon utilization in an air-bridge thermophotovoltaic cell. Nature, 2020.586(7828): p. 237-2415. Lim, J., et al., Enhanced Photon Utilization in Single Cavity Mode Air-Bridge Thermophotovoltaic Cells.ACS Energy Letters, 2023. 8: p. 2935-2939.

Narrow gap semiconductor for IR imaging and sensing : A review

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IR detection and imaging typically require exotic narrow-gap semiconductors to convert photons to electrons. The IR spectrum spans from near-infrared (NIR) photons (close to 1 eV) for smartphone applications and astrophysics imaging, to short-wave infrared (SWIR, 800 meV) for industrial control, mid-wave infrared (MWIR, 250 meV), and long-wave infrared (LWIR, 130 meV) for defense imaging, up to very long-wave infrared (VLWIR, 80 meV) for atmospheric monitoring from space. This broad range necessitates different material systems with specific features tailored to various applications. For instance, IR imaging devices for defense require high performance and stability but in modest volumes, whereas imaging for smartphones prioritizes lower costs due to large-scale production. Conversely, sensing for space typically involves small series (only a few pieces) but demands ultimate performance with additional requirements for radiation hardness. At CEA-LETI, we develop various material systems for these applications [1], including III-V InGaAs or type-II superlattices (T2SL) based on Sb, as well as II-VI semiconductors such as CdHgTe and its associated substrate CdZnTe, covering the entire IR spectral band. Column IV materials like Ge and GeSn are also being investigated [2] for photonic integrated circuits, specifically targeting growth on Si for large wafers (200-300 mm) and low costs. This presentation will discuss these different material systems in the context of their targeted applications, highlighting the unique specificities of each. The aim is to provide a balanced overview of the current landscape of narrow-gap material systems developed at LETI for IR sensing.

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Functional Development of Unexplored Materials Utilizing Informatics Methods: With a View toward Device Development

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Recent technical advances in materials informatics have enabled unprecedented capabilities for materialsdiscovery and development through screening and selection. These have a beneficial effect on the development ofunexplored material groups. These methods have advanced to the stage of dissemination across various forms ofexperimental research, with active efforts involving experimental researchers. Attempts are being made to introducemachine learning into various forms of materials research, not only for data-driven selection and screening ofcandidate materials expected to have the desired properties, but also for optimizing process parameters andanalyzing and database-forming various measurement results. This presentation introduces our research, which useinformatics approaches to explore novel thermoelectric materials and devices, as described below.– A database of electronic structure parameters of the charge-transfer energy (Δ) and the onsite Coulomb repulsioenergy (U) for 566 transition-metal compounds containing any of 11 anions is constructed. Understanding andcontrolling electronic structure can improve thermoelectric transport properties. High-performance thermoelectrictransition-metal compounds are mainly located in two specific regions in the Δ−U diagram. Attractivthermoelectric materials will be developed by searching for unexplored transition-metal compounds in these two

regions of the Δ−U diagram. [1– An efficient method for optimizing process parameters, a closed-loop thin-film growth method utilizing machine-learning prediction process, was developed. [2,3] It has significantly reduced the number of requiredexperiments to optimize process parameters in thin-film fabrication using a molecular beam epitaxy (MBEapparatus.– Miniaturized thermoelectric devices have been developed with a view toward their application in IoT devicesThese devices are fabricated by microfabricating high-performance thermoelectric epitaxial thin films grown byMBE. Highly reliable device operation has been successfully achieved. A device, containing 36 p-n pairs (71 πjunctions) in a 12 mm square region, generated a maximum output voltage of 0.58 V and a maximum outputpower density of 21 mW·cm−2

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Session: Nanotechnology and Nanoscience

Hybrid Electrode Systems Using Unique Inorganic Materials for Nanoenergy Technology

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We report the fabrication of hybrid electrode systems based on unique inorganic nanomaterials and their electrochemical applications in energy technologies. Coordination polymer (CP*)-derived inorganic materials have been increasingly used owing to their superior electrocatalytic activity and durability. A Zn-based coordination polymer (ZnCP*) is employed to synthesize a bimetallic iron–nickel–nitrogen–carbon (FeNi_NC*) catalyst that serves as an electrocatalyst for both the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER).

The ZnCP* is constructed by incorporating the 2,6-bis[1-(4-carboxyphenylimino)ethyl]pyridine ([N3*]) ligand into a zeolitic imidazolate framework (ZIF). The [N3*] ligand offers strong metal-binding capability owing to its electron-rich nitrogen sites. This coordination facilitates the efficient incorporation of Fe and Ni into the ZnCP* framework, generating a high density of Fe–N x /Ni–N x active sites after pyrolysis. The optimized FeNi_NC* demonstrates excellent electrocatalytic performance.

NiCo layered double hydroxide (NiCo-LDH) and NiCoAl-LDH are electrodeposited onto three-dimensional (3D)-printed electrodes (3D-PEs) prepared by fused deposition modeling (FDM). The 3D-PEs are surface-modified prior to deposition to achieve a high-mass-loading cathode for an asymmetric supercapacitor. The unique 3D-PE architecture ensures efficient ion transport, enabling the fabrication of thick, monolithic electrodes. We also report a self-supported NiCoAl-LDH/graphene aerogel (GA) electrode fabricated via a film- casting–electrodeposition strategy. The GA, consisting of an interconnected 3D porous graphene network, enables rapid electron transport and efficient electrolyte ion diffusion. Moreover, the residual oxygen-containing functional groups on the GA facilitate uniform nucleation and strong interfacial interaction of the LDH nanosheets, thereby enhancing electrochemical performance. The resulting electrode can be used directly without external metallic current collectors or binders.

Creation of Highly Dispersed Ni Nanoparticles with Various Unique Catalysis

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Supported metal nanoparticles have been widely utilized as the heterogeneous catalysts in various chemical processes; however, most of the processes rely on the use of noble metal catalysts, such as Pd, Pt, Rh, etc., which are expensive and limited resources. Thus, the development of supported non-noble metal nanoparticle catalysts is indispensable for realizing sustainable society. In particular, since Ni is a congener of Pd and Pt, which show various catalysis, the development of Ni nanoparticle catalysts with high performance has attracted attention. One of the most challenging issues on the non-noble metal nanoparticle catalysts is preparation of zero-valent active species without aggregation because conventional reduction of supported non-noble metal species like Ni under an H

2 atmosphere requires severe conditions (more than 300 °C) differently from the case of noble metals. To overcome this issue, we made a strategy of utilizing comparatively strong reductants soluble in organic solvents for the reduction of supported Ni species at milder temperatures (below 100 °C). After various investigations, we have successfully prepared highly dispersed Ni nanoparticles supported on CeO 2 (Ni/CeO 2 -reductant) via sodium naphthalenide (NaNaph) or pinacol borane (HBpin) reduction of CeO 2 -supported Ni hydroxide species formed by deposition-precipitation, which were confirmed by comprehensive characterization methods including XAFS, STEM, XPS, CO DRIFT, CO pulse chemisorption, and so on. [1]–[3] It is noteworthy that these Ni nanoparticles exhibited quite high and unique catalytic performances for a variety of organic molecular transformations: decarbonylation of aldehydes with the broadest scope and the highest selectivity among non-noble metal catalysts, [1] dehydrogenative aromatization of various aliphatic compounds including cyclohexanone derivatives for the first time as the non-noble metal catalysts, [2] and the first example of primary benzylic C(sp 3)–H selective dehydrogenative silylation of alkylarenes. [3] Furthermore, we have recently achieved ambient-pressure hydrogenation reactions from aromatic compounds to cycloalkanes and from nitriles to primary amines using Ni/CeO 2 -HBpin without any additives for the first time among non-noble metals. In summary, the new strategy for creation of highly dispersed Ni nanomaterials paved the way to realizing difficult molecular transformations for previous non-noble metal catalysts, which will be applicable to other various non-noble metals and catalytic reactions in the future.

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Why Is Blue Fluorescence generated by Carbon Quantum Dots and Amine-Branched Dendrimers?

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Fluorescence properties of molecules/materials composed of dyes, metals/metal oxide clusters, metal compounds/carbon quantum dots, amine-branched dendrimers, and proteins are effective in photovoltaic, photocatalytic, and photodynamic studies based on light irradiation. This report discusses the characteristics of carbon quantum dots and poly(amido amine) dendrimers that emit blue fluorescence. Carbon quantum dots are particles of 2-4 nm in size, consisting of graphitic cores and terminal groups such as amine and carboxylic acid and emitting strong blue fluorescence [1]. As the amine content increases, the fluorescence intensity rises. Although its semiconductor properties are not particularly strong, when added to dye sensitized solar cells, it effectively serves as a photosensitizer aid. Increasing the amount of amine leads to higher singlet oxygen production, making it a promising drug for photodynamic therapy [2]. At the same time, it has been confirmed to produce photothermal therapy effects. It dissolves easily in water and has good biocompatibility, making it suitable for both nonbio- and bio-based applications.

Poly(amido amine) dendrimer is a dendritic polymer grown with alkylamide as a spacer at the branching point of tertiary amine, and it emits blue fluorescence under an oxygen-rich atmosphere [3]. By complexing with other molecules or materials, it is effective as a fluorescence imaging material.

Because it is water-soluble, biocompatible, and singlet oxygen generatable, its application in photodynamic therapy has been confirmed, but the photothermal therapy effect seen in carbon quantum dots has not been confirmed. The emission of poly(amido amine) dendrimers occurs with time variation under an oxygen atmosphere, but such delays do not occur with carbon quantum dots.

Based on these facts, this report discusses the mechanisms of fluorescence generation of carbon quantum dots and poly(amido amine) dendrimers.

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Structural Effects of Cu Nanoclusters in Electrochemical Nitrate Reduction Reaction toward Ammonia Synthesis

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[Introduction]

Ammonia (NH3) has attracted significant attention as a next-generation fuel for power generation, not only for its use as a fertilizer and chemical feedstock because of its high energy density and its ability to burn without emitting carbon dioxide. The electrochemical nitrate reduction reaction (eNO3−RR) is an promising reaction system because it can convert NO3 – , which is contained in nitrogen fertilizers and industrial wastewater, into NH3 at ambient conditions, thereby restoring the nitrogen cycle, which has been disrupted on a global scale[1]. In addition, metal nanocluster (NC), which is composed of a few to several hundred metal atoms, exhibits unique physical properties that differ from those of ordinary bulk metals, making them highly promising catalysts for various reactions. In the eNO3 – RR system, it has been reported that Cu-based catalysts exhibit high activity, so we focused on employing Cu NCs as catalysts. However, the effect of the structure of Cu NC on eNO3 – RR remain unclear. Therefore, in this study we synthesized two types of Cu14 NC with similar geometric structures but different ligand numbers and revealed the correlation between the geometric structure and eNO3 – RR activity.

[Experiment]

First, we synthesized triphenylphosphine (TPP)/tert-butylthiolate (St Bu) protected Cu14(TPP)7(St

Bu)3H10 (Cu14(TPP)7) [2], and TPP/1-pentanethiolate (SC5H11) protected Cu14(TPP)8(SC5H11)3H10 (Cu14(TPP)8) [3] using liquid-phase reduction. The products were crystallized, and their geometric structures and chemical compositions were confirmed using single-crystal X-ray diffraction (SC-XRD) and electrospray ionization mass spectrometry (ESI-MS). Next, each Cu14 NC was supported on carbon

black (CB) using an impregnation method to prepare the electrocatalysts (Cu14(TPP)n/CB; n = 7, 8). The eNO3–RR activity was evaluated in an 0.1 M KOH aq. Containing 0.1 M KNO3 as the nitrate source.

[Results and Discussion]

ESI-MS and SC-XRD analyses confirmed that controlling the type of thiolate (SR) ligand enabled the synthesis of two Cu14 NC with different numbers of TPP ligands. Transmission electron microscopy (TEM) showed that Cu14(TPP)n/CB (n = 7, 8) was uniformly dispersed on carbon black without aggregation. Electrochemical evaluation of eNO3−RR revealed that Cu14(TPP)7/CB exhibited a Faradaic efficiency for NH3 formation approximately 1.76 times higher than that of Cu14(TPP)8/CB. Structural analysis suggested that this difference originated from variations in the upper Cu-core structure. In Cu14(TPP)8, the bulky TPP ligands induced elongation and distortion of the CuS3P motif, leading to a twisted, low-symmetry structure and reduced stability. These findings indicate that the superior activity of Cu14(TPP)7 arises from 1) the presence of CuS3 motif favorable for NO3− adsorption and 2) its higher structural stability [4].

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Hepatocyte-Specific Nanoparticle for Sensitive and Precise Hepatobiliary Magnetic Resonance Imaging

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Hepatobiliary magnetic resonance imaging (MRI) has been advocated as the most sensitive method for early non-invasive diagnosis of liver tumors in patients afflicted with liver cirrhotic and hepatitis, but its clinical utility has been largely hindered by the lack of sensitive and specific contrast agents (CA). Although nanoparticles have been demonstrated as high-performance CA to overcome these drawbacks, the design of hepatocyte-specific nanoparticle-based CA has long been a challenge because most nanoparticles are likely to be sequestered by Kupffer cells regardless of their surface ligands. Here, we report a sensitive ultrasmall manganese ferrite nanoparticle modified with polyethylene glycol-ethoxy-benzyl ligand on the surface (MnFe2O4-EOB-PEG)- based CA, where synergistic collaboration of the manganese ferrite core and targeting ligand gives rise to superior

hepatocyte specificity, for safe and precision hepatobiliary MRI in large animals, including pigs, rabbits and macaques.We also show that when compared with clinically used gadoxetate disodium, MnFe2O4-EOB-PEG could facilitate faster, ultrasensitive and high-resolution hepatobiliary MRI, providing a significantly improved detection rate (92% versus 48%) for early-staged liver tumors and an even more accurate assessment of biliary obstruction. As a result, biocompatible MnFe2O4-EOB-PEG nanoparticles show great potential for clinical translation as next-generation liver-specific MRI contrast agents.

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Nanoarchitecting Mesoporous Metals: From Single-Component Mesoporous Co to Single-Crystalline High-Entropy Alloys

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In situ-grown amorphous oxide trilayer for self-rectifying resistive switching

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RRAM-based crossbar arrays can perform data storage and computation in the same physical hardware, providing a route for next-generation in-memory computing [1] . However, the absence of intrinsic rectification gives rise to sneak-path currents, while an insufficient resistance ratio between the high-resistance state (HRS) and low-resistance state (LRS) reduces the read margin and limits readout accuracy. Incorporating a switching device, as in one-transistor-one-resistor (1T1R), can improve cell selectivity [2] . However, the additional switching component increases the cell footprint and fabrication complexity, thereby limiting the integration density and scalability of crossbar arrays [3] . Consequently, self-rectifying two-terminal RRAM devices are highly desirable for selector-free active crossbar circuits [4] . This talk introduces a self-rectifying Schottky structure comprising an oxide trilayer grown in situ by room- temperature radio-frequency sputtering deposition. Based on our previous work [4] , the Ni/Ta 2 O 5 interface forms a relatively high Schottky barrier, while the Ta 2 O 5 /IGZO heterointerface facilitates efficient electron transport under forward bias via thermionic emission over the conduction-band offset, with the population of transport-active electrons determined by the Fermi-Dirac distribution. An oxygen-deficient CuO x layer inserted between Ta 2 O 5 and IGZO creates a trap-rich region that promotes space-charge-limited conduction. To evaluate the dimensional scalability of this architecture, crossbar devices with lateral dimensions ranging from hundreds of micrometers to the sub-micrometer scale are fabricated. DC measurements reveal

reproducible self-rectifying resistive-switching hysteresis, with a rectification ratio exceeding 10 5 and an HRS/LRS resistance ratio more than 10 3 following optimization of the SET voltage. In addition, the resistance ratio is evaluated at elevated cell temperature, ranging from 20 °C to 70 °C, to confirm the temperature-dependent characteristics. The same devices are characterized using rectangular AC voltage waveforms. The reverse current in the third quadrant is effectively suppressed, while the first-quadrant response exhibits conductance-state-dependent memristive behavior. These results demonstrate that the in situ-grown oxide trilayer enables resistive switching and intrinsic current rectification within a single two- terminal device. The proposed structure therefore provides a promising platform for high-density, selector-free 1R crossbar arrays for in-memory computing.

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Channel-length scaling effects on the electrical performance of top-gate In-Ga-Zn-O thin fil transistors

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Oxide semiconductor thin-film transistors (TFTs) have been widely adopted in display backplanes owing to their cost-effective fabrication and relatively high electron mobility [1, 2] . Among various TFT architectures, the self- aligned top-gate TFT architecture offers relatively low parasitic capacitance and requires fewer photomasks [3] , making it promising for high-resolution displays [4] . Displays with resolutions beyond current standards require increasingly compact pixels and, consequently, short-channel TFTs. However, channel-length scaling effects on the electrical performance of self-aligned top-gate IGZO TFTs remain insufficiently understood.

In this work, channel-length scaling effects in self-aligned top-gate IGZO TFTs are investigated. The devices are fabricated using industry-compatible processes, including sputtering, chemical vapor deposition, and conventional photolithography. The channel length varies from several tens of micrometers down 2 μm. Transfer and output characteristics are measured over a range of device

temperatures from 20 °C to 70 °C. To evaluate the scaling effects, the effective field-effect mobility (μ eff), subthreshold swing (SS), and early voltage (V A) are extracted from the measurements. The extracted μ eff remains nearly constant at relatively long channel lengths but decreases to below 10 cm 2 /V·s at a relatively short channel length. It results from the source/drain contact resistance accounts for an increasing fraction of the total resistance. As the device temperature increases, thermal activation of electrons from localized states enhances subthreshold conduction, while the temperature-dependent thermal component of SS also increases. Consequently, SS increases with temperature, with the measured degradation being more pronounced in relatively long-channel devices. In the on-state, μ eff decreases with increasing temperature, which is consistent with enhanced phonon scattering and a reduction in the carrier momentum-relaxation time. Furthermore, the magnitude of the V A decreases at shorter channel lengths, indicating remarkable channel-length modulation and lower output resistance.

Overall, simply reducing the channel length can introduce substantial performance penalties in future displays with resolutions beyond UHD. These findings highlight the need for novel short-channel TFT architectures that minimize contact-resistance and channel-length-modulation effects while maintaining high effective mobility, steep subthreshold switching, robust current saturation, and thermal stability.

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Characterization of Joule Heating in Submicron Metal Lines

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Yamauchi ERATO Public Symposium: How Next-Gen "Holey Materials" Will Transform Our Lives (Co-Sponsored by International Research Unit, Nagoya University)

Poster Presentations

Sustainable Ir-catalyzed Hydroaminimethylation of Olefines with Formic Acid as H 2 - source via Ligand Architecture Tuning

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Hydroaminomethylation, defined as a one-pot amine synthesis protocol from olefins via three-step tandem reaction including hydroformylation, condensation and imine-hydrogenation, is advantageous with high atom economy, operational simplicity, and low-cost raw materials [1]. Compared to Rh-catalyst with high cost and resource scarcity, the relatively inexpensive Ir-one has attracted much attention, in which the phosphine ligands with distinct stereo-electronic properties play predominant role in tuning the performance of the catalyst. However, in Ir- catalyzed hydroaminomethylation, the side-reactions of olefin-hydrogenation/isomerization happens universally while using syngas (CO/H 2) as the reactant. Hence, H 2 O or formic acid (FA, HCOOH) is often applied as potential H 2 -source to avoid the presence of high-pressure gaseous H 2 [2,3]. Herein we reported firstly the synthesis of steric-bulky mono-phosphine (L1) and its ionic counterpart (L2), in which the sterically bulky quaternary carbon-centered moiety substituted by three phenyl-groups was neighbored to PPh 2 -fragement, to utilize the unique architecture of the phosphines to tune the performance of Ir-catalyst while using HCOOH as a masked H 2 -source to generate H 2 in situ for hydroaminomethylation. Emphatically, compared to the conventional PPh_3, L1 exhibited superior air/moisture insensitivity and thermal stability (T decomp. >300 o C). Due to the available intramolecular P□□□H acid-base pair (P□□□H length, 2.22 Å, confirmed by the single crystal X-ray diffraction characterization), the P-atom in L1 is fixed in the cavity of surrounding phenyl/imodazolyl-rings against the attack by H 2 O or O 2 , warranting the good stability of L1. Resultantly, L1 enbled $[Ir(COD)Cl]_2$ to be highly active, selective and stable catalyst, which was subjected to 10-run recycling uses without activity loss. The in situ high-pressure FT-IR and ^1H NMR spectroscopic studies disclosed that the facilitated formation and stability of the Ir-H active intermediate in L1-$[Ir(COD)Cl]_2$ system was responsible for the observed superior catalytic performance.

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Detachable Block Copolymer Distributed Bragg Reflectors for Wavelength-Matched SERS Sensing

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The sensitivity of surface-enhanced Raman scattering (SERS) depends strongly on how closely the working wavelength of the plasmonic substrate matches that of the Raman laser. Most approaches tune this match by adjusting the size and shape of the metal nanoparticles. We instead recycle the incident photons using a distributed Bragg reflector (DBR) fabricated by block copolymer self-assembly and attached to the SERS substrate as a separate, interchangeable component.

A compositionally symmetric polystyrene-b-poly(2-vinylpyridine) (Mn = 82 kDa, Đ = 1.05) was annealed on PS- brush-grafted glass into defect-free lamellae aligned parallel to the substrate under symmetric confinement, with an interlamellar distance (L0) of 52.1 nm. Partial crosslinking of the 2VP units with 1,4-dibromobutane, followed by soaking in lactic acid, swelled only the P2VP microdomains. The crosslinking density controls how far these domains swell, so L0 could be tuned up to 301 nm, 5.78 times the pristine value, while small-angle X-ray scattering peaks at q/q* = 1:2:3:4:5:6 confirmed that the parallel multilayer order survived this expansion. Reflected wavelengths calculated from the Bragg–Snell relation spanned 498–880 nm and agreed with measured reflectance spectra within 1 %, and a 2 μm film reflected 76 % at 498 nm with a peak width of 19.1 nm.

To build the sensor, we deposited Au nanoparticles of 18 ± 2 nm on a flexible, transparent cellulose nanofiber film, giving an absorption maximum at 521 nm. Encapsulated DBR films were placed beneath this substrate without any adhesive layer, so the working wavelength (λw) could be changed simply by exchanging the reflector. Scanning λw located a maximum at 522 nm: the Rhodamine 6G intensity at 610 cm−1 increased approximately 99- fold relative to the substrate without a DBR, the limit of detection improved from 10−7 to 10−9 M, and the enhancement factor reached 1.13 × 106, with a spot-to-spot relative standard deviation of 7.06 %. For the pesticide thiram, the detection limit fell from 10−5 to 10−8 M, and 0.2 ppm was detected directly from the skin of contaminated apples, well below regulatory residue limits. Because the reflector is a separate component, the working wavelength can be retuned by exchanging the DBR film alone rather than rebuilding the whole device.

This offers a practical route to on-site sensing for food safety and environmental monitoring.

Analysis of Ammonia Dispersion and Water Curtain Mitigation Following a Safety Valve Release from an Ammonia Storage Tank

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Ammonia has attracted considerable attention as an alternative energy carrier capable of overcoming the structural limitations of hydrogen energy systems, leading to the expansion of port infrastructure for its storage and handling. However, large-scale ammonia is stored in atmospheric-pressure, cryogenic storage tanks, and a malfunction of the cooling system may increase the internal pressure, resulting in the release of ammonia through a safety valve. Such accidental releases pose significant risks to human safety and the surrounding environment.

In this study, the dispersion characteristics of ammonia at different concentration levels and the physical mitigation effect of a water curtain following a safety valve release from a large-scale ammonia storage tank were investigated using the computational fluid dynamics (CFD) code OpenFOAM. The numerical model was first validated against the INERIS and Champclauson experiments and then applied to a leakage scenario based on an actual port environment. The simulation results showed that low-concentration ammonia plumes dispersed upward and horizontally before remaining near the ground surface for an extended period. In contrast, high-concentration plumes exhibited both horizontal transport and upward dispersion, while downward dispersion was not observed. Ammonia concentrations within the flammable range maintained a relatively stable dispersion pattern in the upper layer during the release and rapidly disappeared immediately after the release ceased. When a water curtain was installed near the safety valve, horizontal plume dispersion was effectively suppressed and redirected upward, significantly reducing the exposure risk associated with high-concentration ammonia. These findings suggest fundamental data for the safety design of ammonia storage facilities and the development of effective water curtain operation strategies.

Keywords: Ammonia, Dispersion Characteristics, Mitigation Effect, Safety Valve, Water Curtain, Computational Fluid Dynamics (CFD)

[Acknowledgment]

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Effect of Laser Polishing Process Parameters on the Surface Roughness of Martensitic420J2 Stainless Steel

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Laser-based surface polishing is a promising non-contact finishing method that offers precise control of processing parameters and good process reproducibility compared with conventional mechanical and electrochemical polishing methods. This study investigated the effect of laser-processing parameters on the surface roughness of martensitic stainless steel (STS420J2), which is widely used for precision machine parts and tooling. Surface roughness evolution was evaluated as a function of laser power, repetition frequency, scanning speed, point- to-point (P-to-P) distance, and track pitch.

Experiments were performed using a pulsed fiber laser system with a wavelength of 1064 nm, pulse duration of 35–75 ns, focal length of 500 mm, and focal spot diameter of 93 µm. The arithmetic mean surface roughness (Ra) of the specimens was measured before and after laser irradiation using a confocal optical microscope. The specimens were mechanically polished prior to laser treatment. Specimens A and B exhibited initial Ra values of 0.2 ~ 0.3 µm and 1.0 ~ 1.1 µm, respectively.

For Specimen A, the greatest observed roughness reduction, 22.0%, was obtained using a laser power of 50 W (25%), a scanning speed of 4000 mm/s, a repetition frequency of 200 kHz, and P-to-P distance and track pitch values of 0.02 mm. Under the same conditions except for a laser power of 60 W (30%), Specimen B showed a roughness reduction of 18.6%. These results indicate that laser polishing can improve the surface finish of STS420J2 and that the initial surface condition should be considered when selecting laser-processing parameters.

Keywords: Laser, Polishing, STS420J2, Martensitic, Stainless steel

Giant Piezoresponse in Nanoporous (Ba,Ca)(Ti,Zr)O3 Thin Films Enabled by Pore-Induced Lattice Strain

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Lead-free piezoelectric materials with high electromechanical performance are strongly desired for next- generation sensors, actuators, and energy-harvesting devices. Although Pb(Zr,Ti)O3 (PZT) and related Pb-based materials exhibit excellent piezoelectric properties, their toxicity has driven intensive efforts to develop environmentally sustainable alternatives [1]. Among them, Ca/Zr co-doped BaTiO3, (Ba,Ca)(Ti,Zr)O3 (BCZT), is a promising candidate because of its enhanced piezoelectricity near the morphotropic or polymorphic phase boundary [2]. Beyond conventional composition and crystal-structure engineering, nanoscale morphology offers another route to control ferroelectric properties

through local strain [3,4]. Here, we demonstrate that a nanoporous architecture induces exceptionally large lattice strain and a giant piezoresponse in lead-free (Ba0.85Ca0.15)(Ti0.9Zr0.1)O3 thin films.

Nanoporous BCZT films were fabricated by a sol–gel-based soft-templating method using polystyrene-block-poly(ethylene oxide) (PS-b-PEO) as a pore-directing agent. After calcination at 650 °C, elongated nanopores surrounded by highly crystallized BCZT frameworks were obtained. X-ray diffraction confirmed the perovskite phase, while annular dark-field scanning transmission electron microscopy and elemental mapping verified the incorporation of Ca and Zr into the BaTiO3 lattice.

The effect of the nanoporous structure on local lattice deformation was investigated by high-resolution scanning transmission electron microscopy combined with geometric phase analysis. The local strain in the nanoporous BCZT film exceeded approximately 30%, whereas that of the nonporous BCZT film was approximately 0.3%. Thus, pore formation produced a nearly two-order-of-magnitude enhancement in local strain, demonstrating that the pore-wall geometry generates intense lattice distortion. The observed correspondence between the enlarged strain field and the enhanced piezoresponse indicates that nanoscale pore-induced deformation is a key factor governing the electromechanical response. Piezoresponse force microscopy further revealed a remarkable enhancement in electromechanical response. The nanoporous BCZT film exhibited a remanent d33 of approximately 7500 pm V−1, more than ten times larger than the approximately 550–600 pm V−1 obtained for the nonporous film. Clear 180° phase switching and d33–voltage hysteresis behavior were also observed. In addition, the nanoporous film exhibited a dielectric constant of approximately 1500, compared with approximately 1000 for the nonporous film, while maintaining relatively low dielectric loss and adequately low leakage current density.

The enhanced piezoresponse is attributed to pore-induced anisotropic stress and the associated distortion of the BCZT lattice, which promote polarization and electromechanical deformation. Importantly, the enhancement was achieved simply by introducing nanoscale porosity without constructing more complicated nanowire, nanofiber, or core-shell architectures. These results demonstrate that nanoscale morphology and pore-derived strain can serve as effective materials-design parameters, complementing conventional composition- and crystal-structure-based approaches. Nanoporous BCZT therefore provides a simple strategy for developing high-performance lead-free piezoelectric thin films for sensing, actuation, dielectric capacitors, and high-density energy-harvesting applications.

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Thermomechanical and optical properties of germanotellurite glasses doped with Ho 3+ and co-doped with Ho 3+ /Yb 3+ /Tm 3+

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The investigated material is holmium-doped germanotellurite glass (55-x)GeO 2 -30TeO 2 -10SrF 2 -5Nb 2 O 5 - xHo 2 O 3 (GTSN:Ho; x = 0.4% and 2%) and samples of such glass co-doped with Yb3+/Tm3+ ions with the following molar composition: (55-x-y)GeO 2 -30TeO 2 -10SrF 2 -5Nb 2 O 5 -xHo 2 O 3 - yYb 2 O 3 (GTSN:Ho,Yb; x = 0.4%, y=2%) and (55-x-y-z)GeO 2 -30TeO 2 -10SrF 2 -5Nb 2 O 5 -xHo 2 O 3 - yYb 2 O 3 -zTm 2 O 3 (GTSN:Ho,Yb,Tm; x = 0.4%, y=2%, z=0.4%).

To verify the potential applications of the produced glasses, their thermomechanical and optical properties were examined. Differential thermal analysis (DTA) confirmed their desirable mechanical strength, favourable thermal properties, and very good resistance to devitrification. The optical properties of the glasses were studied with a view to their spectroscopic properties and potential applications in near-infrared optical amplifiers and luminescence thermometry (in broad spectral ranges and at elevated temperatures up to 650 K). It was found that in the visible spectral range, the excitation energy primarily initiates the emission of holmium 5 S 2 - 5 I 8 emission with 98 % excellent color purity. Taking into account the significant energy transfer from Yb ions to Ho and Tm ions, it was also possible to develop a temperature measurement model based on the intensity between the anti-Stokes luminescence bands from 5 F 5 (Ho) and 3 F 3,2 / 3 H 4 (Tm) levels, achieving a relative sensitivity of about 1.07%K -1 .

Methodology for measuring Joule heating from electrical power dissipation

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Shrinking device dimensions sharply increases current density at a given operating current, making Joule self- heating non-negligible [1] . Under steady-state conditions, the associated electrical power dissipation produces a temperature rise governed by the thermal resistance of the substrate and

surrounding heat-flow path, thereby altering temperature-dependent transport properties and, consequently, integrated-circuit operation [2] . Quantifying Joule heating is therefore essential for heat-sink and package design and for device-level thermal management.

This work presents a compact, low-cost platform for monitoring Joule-heating-induced temperature changes in electrically biased devices. The platform integrates a T-type thermocouple, a MAX31856 thermocouple-to-digital converter, and an Arduino microcontroller. The thermocouple generates a Seebeck voltage of approximately 40 μV/K [3] . The MAX31856 conditions and digitizes this low-level signal, performs cold-junction compensation, and applies on-chip ITS-90 linearization [3, 4] . The Arduino reads the resulting temperature data through an SPI interface and streams them to a PC for continuous logging. The device substrate is mounted on an aluminum heat- sink plate, and a bead thermocouple embedded in a machined hole monitors the plate temperature. This measurement provides the heat-sink boundary condition for the thermal model. With the effective heat-transfer area A eff defined by the model, the heat flux is evaluated as q'' = Q/A eff , where the heat flow is inferred from the dissipated electrical power, P diss = IV. The platform is demonstrated through measurements of Joule-heating-induced temperature rises in patterned metal lines and semiconductor devices under representative operating conditions.

Combining the measured boundary temperature with the thermal model enables heat flow to be tracked and junction-temperature rise in semiconductor devices to be estimated as a function of dissipated power and operating condition.

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Dendrite-Free Lithium Metal Cycling Enabled by a new novel Ionic Additive

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Lithium metal batteries (LMBs) have emerged as a next-generation energy-storage technology due to their exceptionally high theoretical specific capacity and low electrochemical potential. Nevertheless, their practical implementation remains hindered by uncontrolled dendrite growth, unstable solid electrolyte interphase (SEI) formation, and rapid electrolyte consumption during long-term cycling.

In this work, we report lithium nanographenide (LNG), a graphene-derived ionic compound, as a highly effective electrolyte additive capable of stabilizing lithium metal interfaces at an extremely low concentration. Incorporation of LNG into a conventional 1 M $LiPF_6$ carbonate electrolyte significantly improves ion transport behavior by considerably elevating the lithium-ion transference number. This enhancement promotes uniform lithium deposition and suppresses anion-driven concentration polarization, which is a key factor in dendritic growth. Symmetric Li/Li cells containing the LNG additive exhibited exceptional cycling stability, maintaining low overpotential for several hundred cycles and demonstrating improved resistance against short-circuit failure even under higher current densities. Li/Cu half- cell analysis showed increased Coulombic efficiency and smoother metallic lithium morphology, indicating a more stable and compact SEI formed in the presence of LNG. Electrochemical impedance spectroscopy further confirmed that the LNG-modified electrolyte maintains substantially lower interfacial resistance throughout prolonged cycling. Full-cell tests with NCM layered oxide cathodes revealed that the LNG additive more than doubled the cycle life to reach 70% capacity retention compared to the pristine electrolyte. Additionally, enhanced rate capability was observed across all C-rates, with markedly improved performance at high current densities. These results indicate that LNG offers an effective interfacial-regulation approach that enables practical and electrochemically stable high-energy lithium metal batteries.

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Development of a Corrosion Testing and Evaluation Method for Metallic Materials Considering Ammonia Handling Environments

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Ammonia has considerable potential as a hydrogen carrier and carbon-free fuel. However, because of its high toxicity and strong irritant properties, leakage during storage, transportation, or handling may cause serious harm to human health and the environment. In particular, metallic materials used in pipelines, storage tanks, and transportation equipment may undergo corrosion, pitting, and stress corrosion cracking during prolonged exposure to ammonia due to the effects of moisture, oxygen, temperature, and applied stress. Such damage can reduce the mechanical integrity and leak-tightness of the equipment, thereby increasing the risk of ammonia leakage accidents.

This study aims to address the limitations of existing international standards and establish a corrosion testing and evaluation framework for metallic materials under realistic liquid- and gaseous-ammonia handling environments. In this study, the test conditions and evaluation methods specified in international corrosion testing standards, including relevant IMO guidelines, ISO 7539-2, ISO 16540, and ASTM G31, were comparatively analyzed. The advantages and limitations of the existing standards, as well as their applicability to actual ammonia handling environments, were reviewed. Based on this analysis, a corrosion testing and evaluation procedure applicable to base-metal and welded specimens used in ammonia service was established. The test conditions consisted of two liquid-ammonia conditions and four gaseous-ammonia conditions. Constant strain was applied using a four-point bending method to evaluate susceptibility to stress corrosion cracking. Pitting depth, mass loss, surface appearance, microstructural changes, and damage to welded regions were also comprehensively analyzed.

The results are expected to provide fundamental data for material selection, structural integrity assessment, and leakage prevention in ammonia storage, transportation, and handling facilities.

Furthermore, the proposed method may contribute to the future standardization of corrosion testing methods for ammonia service and the development of relevant industry standards.

Keywords: ammonia transportation, metallic materials, corrosion, stress corrosion cracking, material compatibility

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Sulfonated Fe-MOF–Polytriazole Hybrid Membranes with Enhanced Proton Conductivity: Structure–Property Relationships and Application Potential

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Proton exchange membranes (PEMs) are critical components in fuel cells and other electrochemical energy devices, where they function as ion-conducting barriers separating electrodes while facilitating proton transport. The performance of PEMs depends on achieving high proton conductivity, excellent oxidative stability, controlled water uptake, and robust mechanical properties.

In this work, we report the design and fabrication of advanced hybrid membranes based on sulfonated polytriazole (PTSF) matrices incorporating sulfonated iron-based metal–organic frameworks (Fe-MOFs). The Fe-MOF precursor was synthesized via solvothermal reaction of $FeCl_3 \cdot 6H_2O$ with 2-aminoterephthalic acid, forming Fe-MIL-53-NH_2, which was subsequently post-functionalized through ring-opening sulfonation using 1,3-propane sultone. This sulfonated Fe-MOF (Fe-S MOF) introduces abundant $–SO_3H$ groups, enhancing hydrophilicity and providing potential proton-conducting sites.

The Fe-S MOF was homogeneously incorporated into the sulfonated polytriazole matrix via a solution blending method to prepare free-standing, flexible membranes with varying Fe-S MOF loadings (3–9 wt%). Detailed characterization confirmed successful synthesis and integration of the hybrid membranes. ATR-FTIR and XRD analyses verified chemical modifications, while SEM, AFM, and TEM imaging revealed uniform MOF dispersion and well-separated phase morphologies within the polymer matrix. Thermal and mechanical testing demonstrated that the hybrid membranes retained high oxidative stability and good dimensional stability. The inclusion of sulfonated Fe-MOF improved water uptake (up to 38% at 80 °C) while maintaining controlled swelling ratios (7–15% at 80 °C). Importantly, proton conductivity was significantly enhanced, with maximum values reaching approximately 80 mS cm^{-1} at 80 °C, surpassing the pristine PTSF membrane. The improved proton transport can be attributed to the formation of interconnected ionic channels facilitated by the uniformly dispersed MOF nanoparticles and their hydrophilic domains.

These results demonstrate that the sulfonated Fe-MOF/PTS hybrid membranes offer an effective strategy for designing next-generation PEM materials. By balancing conductivity, stability, and processability, these materials show strong potential for use in fuel cells and other electrochemical devices requiring efficient ion-conducting membranes.

Entropy-Laddered High-Entropy Materials for Reliable Electrochemical Energy Storage Across Wide Temperatures

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The development of reliable electrochemical energy storage systems for operation under variable and extreme temperature regimes requires electrode materials that retain redox activity, rapid charge-transfer kinetics, and structural integrity beyond conventional ambient conditions. High-entropy materials provide a promising platform for addressing these requirements because their multicomponent compositions offer diverse redox-active centers, tunable electronic environments, lattice distortion, and entropy-assisted structural stabilization. Here, we present an entropy-laddered materials design strategy that systematically progresses from unary to high-entropy spinel oxides (U2HESOs) and sulfides (HESs), followed by their integration with conductive two-dimensional MXene nanosheets to enhance electrochemical performance and operational stability across a wide temperature range. The entropy-ladder concept initially establishes a controlled progression from low-component compositions to multicomponent high-entropy frameworks. In the oxide system, sequential incorporation of different metal species into spinel-type structures enables direct examination of how increasing compositional complexity influences phase formation, charge-transfer behavior, and electrochemical durability. The optimized HESO ((CrFeNiZn)Co 2 O 4), exhibits enhanced charge-storage characteristics and retains approximately 82% of its initial electrochemical response after 5,000 cycles. An asymmetric device based on the optimized HESO delivers an energy density of 5.32 Wh kg -1 at 500 W kg -1 under ambient condition. Similarly, the concept is extended to multimetallic sulfides, where entropy engineering is combined with structural regulation to generate nanocrystalline architectures with accessible electroactive sites and shortened ion-transport pathways. The HES system further develops a porous yolk-shell morphology that provides internal void space for electrolyte penetration and accommodates structural variation during repeated electrochemical reactions. The optimized HES (ZnMnNiVCoS) electrode delivers a specific capacitance of 604.53 F g -1 at 1 A g -1 and retains 92% of its initial capacitance after 5,000 cycles.

Beyond room-temperature performance, the electrochemical behavior of these high-entropy materials is examined under a broad range of thermal conditions. Temperature-dependent electrochemical performance measurements are used to evaluate changes in charge-storage behavior, ion transport, interfacial resistance, and electrochemical reversibility. The entropy-stabilized frameworks maintain electrochemical activity under sub-zero, ambient, and elevated-temperature conditions, demonstrating the potential of compositional complexity to support structural and electrochemical resilience. Developed HESO and HES-based devices sustain electrochemical operation from -30 to 80 °C, highlighting their potential for energy storage systems over wide-temperature range.

Despite these advantages, standalone HESO and HES remain constrained by limited electronic conductivity and interfacial resistance during prolonged electrochemical cycling. To address these limitations, the optimized high- entropy materials are integrated with two-dimensional MXene, creating HESO-MXene and HES-MXene hybrid architectures. MXene provides highly conductive electron-transport pathways, large interfacial areas, and accessible ion-transport channels, while the high-entropy phases contribute multimetallic redox activity and entropy-stabilized electroactive structures. Their interfacial coupling suppresses particle aggregation, reduces charge-transfer resistance, facilitates electrolyte accessibility, and improves structural integrity during repeated charge-discharge processes and thermal variation. Overall, this work demonstrates a progressive materials design framework that advances from entropy-laddered compositional engineering for wide-temperature electrochemical validation and subsequently to MXene-assisted interfacial engineering. The combination of high-entropy design with conductive two-dimensional architecture provides a promising pathway toward electrochemical energy storage systems with enhanced charge transport, cycling durability, and thermal resilience for transportation, renewable-energy systems, portable electronics, and other demanding operating environments.

Skin-conformal nanofiber-based adhesive electronics with octopus-inspired 3D suction cups for enhanced transdermal delivery

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Transdermal drug delivery (TDD) systems have evolved, with skin electronics emerging as a technology capable of enabling efficient drug administration. However, conventional skin electronics often rely on rigid materials and expensive fabrication processes, limiting flexibility and skin-adhesion. In this study, we developed cellulose nanofiber (CNFs)-based adhesive electronics by integrating a three-dimensional octopus-inspired architecture (OIA) and a conductive layer. The OIA imprinted on CNFs enhanced adhesion by leveraging the synergistic effect of its adhesive structure and the ability to remain stable even after absorbing active ingredient solutions. Unlike conventional fiber-based TDD platforms, the optimized CNFs-OIA retains its architecture, enabling suction-based adhesion to improve skin attachment. To further enhance the TDD efficiency, we integrated a conductive layer into the CNFs-OIA. This conductive interface generates microcurrents that reduce the electrical resistance of the stratum corneum and facilitates the ionization of active ingredients, thereby improving skin penetration. This study was published in: npj Flexible Electronics 9. 1, 54 (2025).

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Effective HA-Loading Strategy in Internal Dome-Assisted Suction Cups for Enhanced Transdermal Delivery Under Vertical Adhesion and Vibration

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To achieve effective transdermal delivery, it is crucial to overcome the stratum corneum (ST) barrier and maintain high delivery efficiency even on curved, moist, and dynamically moving skin. In response, transdermal delivery technologies have evolved to integrate external stimuli with skin adhesive patch systems [1, 2]. However, conventional approaches frequently depend on painful needle-based injections or cumbersome electronic devices.

Furthermore, most adhesive skin patches exhibit limited transdermal delivery efficiency and suboptimal adhesion, particularly under dynamic skin conditions, thereby constraining their practical applicability. In this study, we present a hyaluronic acid (HA)-loaded suction cup patch with an internal dome structure (HA@d-SC), inspired by the suckers of octopuses, to enhance transdermal delivery under dynamic skin conditions. The internal dome increases the skin contact area, ensuring robust adhesion and temporarily deforming the ST to facilitate efficient HA delivery [3]. HA@d-SC is fabricated using a rapid and precise inkjet printing based liquid loading platform, maintaining consistent delivery and adhesion even under challenging conditions such as vertical application and mechanical vibration. Furthermore, clinical trials demonstrate its potential to improve skin conditions without causing irritation. These findings suggest that HA@d-SC can serve as a versatile platform for therapeutic applications, extending beyond cosmetics when combined with other bioactive agents.

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Discovery of a Physicochemically Robust Co-reactant for Reliable Electrochemiluminescence

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Electrochemiluminescence (ECL) assays depend on co-reactants to generate reliable signals, yet the physicochemical properties of commonly used co-reactants can limit their suitability for biosensing. ri-n- propylamine (TPrA), although widely used, is hydrophobic, susceptible to oxidative degradation, and typically handled as a volatile liquid, which can hinder reproducibility and practical use in bioanalytical workflows. Here, we introduce 4-(dimethylamino)pyridine (4-DMAP) as an alternative ECL co-reactant with physicochemical properties that are inherently better suited for aqueous and biologically relevant environments.

Unlike TPrA, 4-DMAP is a chemically stable solid powder with high aqueous solubility, enabling accurate handling, homogeneous solution preparation, and consistent concentration control. In a tris(bipyridine)ruthenium(II) [Ru(bpy)3]2+-based ECL system, 4-DMAP functions through electrochemical oxidation of its amine moiety, while the conjugated pyridine nitrogen stabilizes the resulting reductive radical intermediate, leading to efficient and reproducible ECL generation.

The practical advantages of 4-DMAP were demonstrated in ECL-based immunoassays, including the detection of protein markers in extracellular vesicles from cancer patient plasma and the measurement of neutralizing antibodies against SARS-CoV-2 in human saliva. Collectively, these results highlight the importance of co-reactant physicochemical properties in ECL assay design and establish 4-DMAP as a robust and user-friendly alternative to TPrA for bioanalytical applications.

Anisotropic Characterization of Makino Bamboo/Epoxy Composites: Fiber Volume Fraction Effects and Transverse Strength Modeling

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Bamboo fiber has gained significant attention as a sustainable reinforcement due to its renewability, low density, and high specific mechanical properties. However, literature remains limited regarding the systematic characterization of the anisotropic elastic and strength behavior of unidirectional bamboo fiber composites across varied fiber volume fractions (v f). This study addresses this critical gap by fabricating unidirectional Makino bamboo (Phyllostachys makinoi) fiber/epoxy composites via resin transfer molding. A comprehensive multi-axial property database was established through a series of tensile, compressive, and off-axis tensile tests. Experimental results demonstrate that longitudinal and transverse moduli and strengths generally increase with v f under both tension and compression, hereas the in-plane shear modulus exhibits a non-monotonic trend. Notably, the transverse tensile strength was the sole property found to decrease with increasing v f . Furthermore, the material displays a pronounced tension–compression asymmetry driven by fiber microbuckling and kink-band formation under compressive loading—a phenomenon rarely quantified in natural fiber composites. To address predictive limitations, this study introduces a linear model that accounts for the fiber's strength contribution in the transverse direction, significantly improving prediction accuracy for transverse strength. Ultimately, this research provides a systematic characterization of volume fraction-dependent anisotropic properties and offers critical insights into the reliability of existing micromechanical models, thereby advancing the material databases and structural design methodologies required for sustainable natural fiber composites.

Policy-Adjusted Economic and Life-Cycle Assessment of Green, Blue, and Gray Hydrogen Production in Australia

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Clean hydrogen is expected to play a central role in achieving global carbon-neutrality targets. This study presents an integrated techno-economic and life-cycle environmental assessment of four hydrogen production pathways in Australia: photovoltaic-powered electrolysis, wind-powered electrolysis, steam methane reforming with carbon capture and storage, and conventional steam methane reforming. The analysis considered 2030, 2040, and 2050 under a net-zero transition scenario. To improve the completeness of the environmental assessment, the life-cycle greenhouse gas emissions embodied in renewable electricity generation infrastructure were explicitly included.

Economic performance was evaluated using the levelized cost of hydrogen (LCOH) and a policy-adjusted, carbon- costed LCOH (C-LCOH), incorporating Australian Carbon Credit Units and the Hydrogen Production Tax Incentive.

By 2050, the median LCOH was estimated at $1.43 kg−1 H2 for photovoltaic-based green hydrogen, $2.14 kg−1 H2 for wind-based green hydrogen, $2.63 kg−1 H2 for blue hydrogen, and $1.78 kg−1 H2 for gray hydrogen. After accounting for carbon costs and policy incentives, the C-LCOH of gray hydrogen increased to $1.97 kg−1 H2, whereas the costs of photovoltaic- and wind-based green hydrogen decreased to $1.42 and $2.09 kg−1 H2, respectively. These results demonstrate that Australian hydrogen policies can improve the cost competitiveness of renewable hydrogen while reducing the economic attractiveness of carbon-intensive production pathways. The findings also highlight that embodied emissions from renewable energy infrastructure should be incorporated into hydrogen certification and policy design to ensure that future support.

Interpretable Machine Learning-Guided Catalyst Design and Process Optimization for Furfural Hydrogenation

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The catalytic conversion of biomass-derived furfural into tetrahydrofurfuryl alcohol (THFA), a high-value chemical intermediate, has attracted considerable attention as a promising pathway toward a sustainable chemical industry. However, identifying effective catalyst compositions and reaction conditions for furfural hydrogenation remains challenging because of its complex reaction pathways and extensive experimental space encompassing catalyst formulation, preparation and pretreatment procedures, and high-temperature and high-pressure operating conditions. Conventional trial-and-

error approaches are therefore time- and resource-intensive. In this study, an interpretable machine learning framework was developed to predict THFA yield and guide the design of catalysts and operating conditions. A literature-derived dataset was constructed by compiling catalyst compositions, preparation and pretreatment parameters, reaction conditions, and experimentally reported THFA yields. Among the evaluated machine learning algorithms, the XGBoost model optimized through grid-search hyperparameter tuning achieved the highest predictive performance, with an R^2 score of 0.958. This result demonstrated the model's ability to capture the complex and nonlinear relationships among catalyst characteristics, preparation parameters, operating conditions, and THFA yield. SHAP (Shapley Additive Explanations) analysis was employed to quantify the contribution of each input variable to the predicted THFA yield. The results revealed that operating variables accounted for a substantial proportion of the model predictions, indicating that precise control of reaction conditions is as important as catalyst composition for achieving high THFA yields. Partial dependence plot analyses were subsequently conducted to elucidate the individual and interactive relationships between major input variables and predicted yield. Based on these analyses, favorable ranges of operating parameters and catalyst preparation conditions were identified. Using the model-derived conditions, 13 bimetallic catalysts were synthesized and experimentally evaluated for furfural hydrogenation to validate the applicability of the machine-learning-guided recommendations. The proposed framework integrates literature-derived experimental knowledge, high- performance prediction, interpretable model analysis, and experimental validation. By systematically linking catalyst characteristics and preparation and operating conditions with catalytic performance, this framework can reduce the experimental search space and accelerate the data-driven development of efficient catalysts for sustainable furfural conversion.

Automated Prediction of Coverage-Dependent Binding Energies for Self-Consistent Microkinetic Modeling

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Mean-field microkinetic models are commonly parameterized on reaction and activation energies evaluated at low or zero adsorbate coverage, despite the strong dependence of binding energies on surface coverage through adsorbate-adsorbate interactions. Explicitly incorporating such effects remains challenging because the number of possible surface-adsorbate configurations increases combinatorically with coverage, making systematic ground state search using density functional theory (DFT) prohibitively expensive.

Here, we develop an automated, data-efficient machine-learning framework for predicting coverage-dependent reaction energetics and integrating them into microkinetic modeling. An equivariant graph neural network machine- learning interatomic potential trained using unrelaxed DFT energetics is first employed to perform Monte Carlo sampling of high-coverage adsorbate configurations. The identified low-energy configurations are selected for DFT structural relaxation, substantially reducing the number of expensive optimizations required to explore the relevant configurational space. The resulting relaxed structures and energetics are then used to train a second machine- learning surrogate model that predicts relaxed adsorption and transition-state energetics directly from initial unrelaxed configurations. The two models are coupled within an active-learning workflow with on-the-fly

refinement, in which training data are iteratively generated for individual elementary reaction steps until free energy landscape for full chemical reaction is achieved.

The framework is demonstrated for thermocatalytic CO 2 hydrogenation on Ni(111) surface, where coverage- dependent energetics are incorporated into microkinetic simulations to predict turnover frequencies and product selectivities under reaction conditions. By combining machine-learning-assisted configurational sampling, active- learning-guided DFT data generation, and surrogate prediction of relaxed energetics, the proposed approach provides a scalable route toward coverage-self-consistent microkinetic modeling while minimizing computational cost and reducing reliance on manually constructed surface configurations.

Heterointerface site-triggered lattice oxygen activation for enhanced alkaline water oxidation

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The oxygen evolution reaction (OER) is a critical step in water splitting and involves a four concerted proton- electron transfer (CPET) process that is subject to a theoretical overpotential limit (~370 mV). This limitation originates from the intrinsic scaling relationship of the adsorbate evolution mechanism (AEM), namely $\Delta G^*OOH = \Delta G^*OH + 3.2 \pm 0.2$ eV. Recently, the lattice oxygen mechanism (LOM) has been proposed as an alternative reaction pathway capable of circumventing this limitation, thereby offering the potential for substantially enhanced OER activity. Previous studies have revealed that sulfides undergo surface oxidation and reconstruction under alkaline electrochemical conditions, particularly in the presence of defects, transforming into oxides or (oxy)hydroxides. Such surface reconstruction is considered a key factor governing catalytic performance; however, the nature of the true active sites and the corresponding catalytic mechanisms remain elusive. In this work, we employ density functional theory (DFT) calculations to investigate the possible OER mechanisms at the heterointerface after surface reconstruction of nickel-doped zinc sulfides with sulfur vacancies under alkaline conditions, with particular emphasis on both AEM and LOM pathways. In this structure, the weakened Zn–O bond strength at the interface induces the generation of non-bonding states, which drives the lattice oxygen to actively participate in the catalytic OER process.

Multifunctional MOF/Glycolipid Nanocomposite Topical Gel for Potent Antimicrobial, Antibiofilm and Wound Healing Activities

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Chronic wound healing remains a major clinical challenge due to persistent microbial infection, biofilm formation, prolonged inflammation, and impaired tissue regeneration. Conventional topical formulations often fail to address these interconnected pathological factors, highlighting the need for multifunctional therapeutic approaches to achieve effective wound healing. In the present study, a multifunctional nanocomposite topical gel was developed using metal-organic frameworks (MOFs) and

Glycolipid (GL) biosurfactant as principal active components, with bioactive compounds incorporated to provide antioxidant and regenerative effects. The optimized MOF/GL nanocomposite was incorporated into a Carbopol-940 based topical gel and systematically evaluated for physicochemical, biological, and in vivo wound healing properties. XRD analysis revealed the successful sequential incorporation of bioactive compounds and GL into the MOF system. FTIR analysis further confirmed the incorporation of bioactive compounds, GL, and Carbopol-940 through characteristic shifts and changes in peak intensities, which might be attributed to hydrogen bonding and electrostatic interactions. The rheological behavior of the gel showed mainly elastic behavior (G' > G"), which signifies the development of a stable network. The amplitude sweep results indicated structural stability with a linear viscoelastic region. The optimized formulated topical gel exhibited good resistance to deformation while maintaining adequate spreading ability. The nanocomposite topical gel exhibited strong antibiofilm and antioxidant activities along with L929 fibroblast cytocompatibility and hemolysis activity. In a 5-mm Wistar rat excision model, the gel markedly accelerated wound closure, achieving significant closure by day 7 without any residual scar. Histological examination revealed enhanced tissue regeneration and restoration of wound architecture, while major organ histopathological evaluation was normal, with no pathological alterations. Overall, these findings demonstrate the potential of the developed multifunctional topical gel formulation for the effective management of chronic and infection-associated wounds.

Synthesis of Chiral Gold Nanostructures on Gold Coral Coated Transparent Conductive Oxide Substrates via [AuCl4]– and Cysteine Interactions for Enhanced Chiral Sensing

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The discrimination of molecular enantiomers is essential in chemistry, biology, and pharmaceutical science because opposite enantiomers can exhibit different biological activities. Surface-enhanced Raman scattering (SERS) offers molecular fingerprint information with high sensitivity; however, distinguishing enantiomers remains challenging because they generally exhibit identical Raman spectra in achiral environments. Chiral plasmonic substrates provide a promising approach by combining SERS enhancement with enantiomer-dependent interactions. Developing accessible fabrication methods and understanding the chemical processes governing chiral growth are therefore important for advancing these sensing platforms. Here, we present a two-step electrochemical strategy for fabricating chiral Au nanostructures on corals Au films supported on indium tin oxide-coated glasssubstrate. Corals Au films were first prepared by block-copolymer-assisted electrodeposition [1,2], followed by the electrodeposition of chiral Au nanostructures using L- or D-

cysteine as chiral additive [3,4]. This sequential electrodeposition approach provides a platform for SERS-based enantiomer discrimination [4]. In the second chiral Au nanostructures synthesis step, the reaction time between cysteine and $[AuCl4]^-$ before electrodeposition strongly affected the resulting chiroptical response. Pronounced circular dichroism (CD) signals were reproducibly obtained after a reaction time of 20 min, whereas prolonged reaction weakened the CD response. Substrates prepared using opposite cysteine enantiomers exhibited opposite CD signals in the visible region. To investigate the chemical origin of this behavior, the precursor solutions were examined using time-dependent CD and UV–vis spectroscopy, nuclear magnetic resonance spectroscopy, and X-ray absorption spectroscopy. The combined results supported chloride-ligand substitution by cysteine and reduction of Au(III), accompanied by changes in the cysteine species. These observations suggest that the evolving coordination environment and oxidation state of the Au precursors as well as oxidation of cysteine play important roles in subsequent chiral nanostructure growth. The synthesized chiral Au/corals Au substrates exhibited stronger SERS responses than other substrates, demonstrating the benefit of integrating the two structured components. Their sensing capability was evaluated using L- and D-phenylalanine in aqueous solution. The resulting spectra displayed enantiomer-dependent intensities, with the preferred response reversing upon changing the chirality of the cysteine used for substrate preparation. These complementary responses demonstrate the potential of the substrates for SERS-based chiral discrimination. References [1] C. Li, Ö. Dag, T. D. Dao, et al., “Electrochemical Synthesis of Mesoporous Gold Films Toward MesospaceStimulated Optical Properties,” Nature Communications 6 (2015): 6608. [2] H. Lim, K. Kani, J. Henzie, et al., “A Universal Approach for the Synthesis of Mesoporous Gold, Palladium and Platinum Films for Applications in Electrocatalysis,” Nature Protocols 15 (2020): 2980–3008. [3] I. Gu, T. Ishida, and T. Tatsuma, “One-Step Electrodeposition of Chiral Plasmonic Gold Nanostructures for Enantioselective Sensing,” Electrochemistry 90 (2022): 077006. [4] K. Nakagawa, J. Wang, T. Zhang, et al. “Synthesis of Chiral Gold Nanostructures on Gold-Coral-Coated Transparent Conductive Oxide Substrates via [AuCl4] – and Cysteine Interactions for Enhanced Chiral Sensing.” Small 22, no. 61 (2026): e75471.

Effect of Cysteine Oxidation Products on the Formation of Electrodeposited Chiral Gold Nanostructures

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Examination of Time-Reversal Symmetry in the Pseudogap of Cuprate Superconductors Using G-HAUP

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Superconductivity emerges at low temperatures and has attracted considerable attention for applications such as ultra-low-loss power transmission and quantum computing. However, the requirement for cooling below the superconducting transition temperature remains a major challenge, motivating the development of superconductors with higher transition temperatures. Among them, cuprate superconductors have been extensively studied because of their high superconducting transition temperatures. Cuprate superconductors exhibit a unique electronic structure called the "pseudogap" in the temperature range between the superconducting transition temperature T_c and the pseudogap temperature T^*, and its origin remains unresolved. Understanding the origin of the pseudogap is important for elucidating the mechanism of superconductivity and for developing superconductors with higher T_c. One prominent hypothesis proposes that magnetic orders, such as loop current order [1] and spin order [2], may be responsible for the pseudogap, and these orders can spontaneously break time-reversal symmetry (TRS). However, previous experimental studies have reported inconsistent results regarding TRS breaking. In this study, we investigate TRS in the pseudogap of the cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) through the reciprocity of its chiroptical properties (optical rotation (OR) and circular dichroism (CD)). Single crystals of Bi2212 were grown using the floating zone method and subsequently vacuum-annealed to obtain underdoped samples with a pronounced pseudogap. The superconducting transition temperature T_c and pseudogap temperature T^* of Bi2212 were determined using a superconducting quantum interference device (SQUID) and angle-resolved photoemission spectroscopy (ARPES), respectively. The wavelength dependence of OR and CD at low temperatures ($T_c < T < T^*$) was measured using a generalized high-accuracy universal polarimeter (G-HAUP). The G-HAUP enables simultaneous and highly precise measurements of OR and CD while accounting for systematic errors arising from optical elements [3–7]. The G-HAUP measurements revealed that both OR and CD exhibit reciprocal sign in the pseudogap of Bi2212. Specifically, the signs of the OR and CD signals remained unchanged when the light propagation direction was reversed. This results are consistent with that observed for right-handed quartz, in which natural optical activity originates from chirality without TRS breaking.

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Transmittance and Coupling Efficiency of Metalenses with Inter-Nanopillar Filling

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Plasma-Induced Surface Engineering of Single Crystalline LiNi 0.5 Mn 1.5 O 4 Cathodes for 5 V- Class Li-ion Batteries

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The growing demand for high-energy-density lithium-ion batteries (LIBs) has renewed interest in 5 V-class cathode materials. Spinel LiNi 0.5 Mn 1.5 O 4 (LNMO) is is a promising cobalt-free cathode owing to its high operating voltage (~4.8 V vs. Li/Li +). Its practical use under high voltage operation, however, is limited by the low electronic conductivity of the ordered phase. The lack of Mn 3+ in the ordered phase suppresses electron hopping, resulting in poor electronic conductivity and limited rate capability. Various cation and anion dopants have been studied to overcome this limitation. Among them, nitrogen has recently attracted attention as a promising anion dopant because it can modify the local electronic structure without significantly altering the bulk crystal structure. Although its potential has been predicted by computational studies, experimental validation remains limited.

In this work, nitrogen was implanted into LNMO using plasma immersion ion implantation (PIII). Ordered LNMO crystals were synthesized by a KCl–LiCl flux method. Field-emission scanning electron microscopy (FE- SEM) revealed an octahedral morphology, and X-ray diffraction (XRD) and Raman spectroscopy confirmed the ordered spinel phase (space group P4 3 32, No. 212). The electrochemical performance was evaluated in CR2032 half- cells. X-ray photoelectron spectroscopy (XPS) showed that the surface nitrogen content of the implanted electrodes increased with the implantation energy, from 3.5 at% to 10.9 at%, indicating that the nitrogen concentration can be tuned by the implantation energy. Sheet resistance measurements and electrochemical impedance spectroscopy (EIS) revealed that moderate implantation reduced both the electrode resistance and the charge-transfer resistance, whereas the highest implantation energy increased the charge-transfer resistance, and the Mn and Ni surface signals in XPS also decreased. The discharge capacity at 0.2C decreased slightly as the implantation energy increased, from 135.4 to 125.0 mAh/g. At 5C, in contrast, both implanted electrodes outperformed the reference: nitrogen implanted LNMO delivered 83.5 mAh/g against 63.5 mAh/g for LNMO, an increase of approximately 31%. These findings demonstrate that nitrogen ion implantation is an effective surface engineering strategy for improving the high-rate performance of ordered LNMO cathodes.

Keywords: Lithium-ion batteries, plasma immersion ion implantation, 5 V-class cathode, nitrogen implantation, high-rate performance

Interfacial Electronic Modulation via Ni Vacancies in Cu2O-NiO for Enhanced C-C Coupling in CO2 Electroreduction

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DAY–3, 11 NOVEMBER, 2026

Session: Energy and Environmental Materials

Chemo-mechanical failure mechanisms in high-performance Li-ion batteries

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Current lithium-ion (Li-ion) batteries do not satisfy the increasing demands of portable electronic devices and electric vehicles, due to low energy densities, safety issues and high cost. High-capacity electrode materials are needed, and researchers have made significant progress over recent years. However, integrating these materials into practical cells has lagged due to several technical challenges. For example, volume expansion of active particles, phase transformation and mechanical stresses generated during cycling may cause cracking, interfacial debonding and poor cycling performance. Up to now, a fundamental understanding of chemistry and mechanics coupling and material failure in high-performance batteries is still lacking.

In this presentation, we like to report our recent work on investigation of chemo-material failure of electrode materials in high-performance Li-ion batteries via operando characterization, mechanical testing, and atomistic modeling. Firstly, we discuss the evolution of microstructure, phase composition, particle size and mechanical stress in Si anodes during charging/discharging cycling and relevant strategies to overcome cracking and pulverization of Si particles [1-4]. Then, we like to report recent work on Ni-rich layered oxide cathodes, including structural evolution, material degradation and possible doping and surface modification techniques to improve the cycling performance and capacity retention [5-7].

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Electrochemical CO 2 Reduction to C 2 H 4 Using Cu-Based Electrocatalysts

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Achieving carbon neutrality is one of the most critical challenges facing humanity today. While expanding the use of renewable energy is undoubtedly essential, it is insufficient on its own. CO 2 emissions originating from chemical reactions in fundamental industries—such as steelmaking, concrete production, and chemical manufacturing—cannot be fully eliminated merely by shifting energy sources. Therefore, the development of direct CO 2 management and utilization technologies is of paramount importance.

Our research focuses on the electrochemical CO 2 reduction reaction (CO 2 RR) as a promising technological pathway, with a specific emphasis on the selective production of ethylene (C 2 H 4). In this presentation, we report on two copper (Cu)-based electrocatalysts that we have developed for C 2 H 4 production with relatively high selectivity. The first catalyst is copper oxide (CuO) prepared on gas diffusion layer (GDL) as the active species. This was fabricated by depositing an alloy onto a gas diffusion layer via sputtering, followed by a specific chemical treatment. This electrode not only achieved a Faradaic efficiency of over 50% for C 2 H 4 production but also demonstrated exceptional long-term durability, successfully maintaining sustained C 2 H 4 generation for several hundred hours.

The second catalyst is ligand-free Cu nanoparticles synthesized through our proprietary chemical process. This catalyst also achieved a Faradaic efficiency exceeding 50% for C 2 H 4 . Notably, it demonstrated high applicability and maintained its excellent C 2 H 4 selectivity even when integrated into a zero-gap cell architecture, which is crucial for practical, industrial-scale applications.

In this presentation, we will discuss the fabrication processes, electrochemical properties, and the mechanisms underlying the high efficiency and stability of these novel Cu-based electrocatalysts.

Defect Engineering in Electrocatalysts for Sustainable Energy Conversion

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Nanostructured materials are essential for advancing energy storage and conversion technologies due to their enhanced electrochemical properties. To fully optimize their performance, understanding and controlling defects at the atomic level is crucial. 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 electrode and electrocatalyst functionalities of nanostructured materials. In this talk, diverse

examples of defect-engineered nanostructures will be presented along with the correlation between chemical bonding nature and energy functionalities. The various roles of crystal vacancies in optimizing the catalyst and electrode performances will be highlighted based on combined in situ/ex situ spectroscopic analyses.

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Sulfided-ZnBiMo heterostructures for the photocatalytic production of hydrogen from water splitting

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One of the most promising methods for producing green hydrogen with zero carbonaceous compounds emissions is the photocatalytic method using semiconductor materials. Among photocatalytic materials, heterostructures of semiconductor materials are attractive for application as potential photocatalysts in the production of green hydrogen from water splitting due to their improved photocatalytic properties such as separation of photogenerated (e - , h +) charges and a lower band-gap energy. In this work, sulfided ZnBiMo-x (s-ZnBiMo-x) heterostructures (x =1.0, 2.0, 3.0

and 5.0 mol % of Mo 6+) prepared by the coprecipitation method were tested in the photocatalytic reaction of hydrogen production from water splitting and using methanol as sacrificial agent. s-ZnBiMo-x heterostructures with a Mo 6+ molar concentration of 3.0 % showed the highest hydrogen evolution after 5 h of photocatalytic reaction using UV light irradiation, which is improved 400.0 % with respect to that obtained with only s-ZnBi heterostructure. Characterization of s-ZnBiMo-x heterostructures by XRD, HRTEM, FTIR, Raman and XPS spectroscopies reveals the presence of sulfided-bismuth carbonate (s-Bi 2 O 2 CO 3) and sulfided-zinc carbonate hydroxide hydrate (s-Zn 4 (CO 3) 2 (OH) 6 .H 2 O) phases at low concentration of Mo 6+ . While, there is appearance of the sulfided-bismuth molybdate (s-Bi 2 MoO 6) phase at Mo 6+ molar concentration higher than 2.0 %, suggesting that CO 3 2- anions are substituted by the incorporation of Mo 6+ O 6 2- anions forming the semiconductor s-Bi 2 MoO 6 phase. UV-Vis experiments reveal that the incorporation of Mo 6+ in the s-ZnBi heterostructure promotes the decrease in the band- gap energy. While, PL studies suggests that sulfur in s-ZnBiMo-x heterostructure promotes highest separation of photogenerated (e - , h +) charges and thereby the inhibition of the recombination rate of electron – hole pairs. It is suggested that s-Bi 2 O 3 CO 3 and s-Zn 4 (CO 3) 2 (OH) 6 .H 2 O and s-ZnBi 2 MoO 6 heterostructures are the main photoactive phases to produce hydrogen from the water splitting.

Rational Design of La-Based Non-Equimolar High-Entropy Metal Oxides for Efficient Oxygen Evolution

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A series of La-based non-equimolar high-entropy perovskite oxides, LaSrCo1-x- yNixFeyO3, together with the parent La00.7Sr0.3CoO3 (denoted as P1), were synthesized via solution combustion method and investigated as oxygen evolution reaction (OER) electrocatalysts in alkaline media. X-ray diffraction confirmed the formation of a single-phase crystalline perovskite structure, while FE-SEM revealed a porous network of interconnected nanoparticles. Among all compositions, the dual-substituted LaSrCo0.5Ni0.12Fe0.38O3 (denoted as P7) exhibited the best OER performance, delivering the highest current density, the lowest onset potential, and excellent stability. P7 also achieved a 3.6-fold higher ECSA-normalized current density than P1, demonstrating the synergistic effect of Ni and Fe dual substitution. High-resolution TEM confirmed homogeneous elemental distribution and successful incorporation of Ni and Fe into the perovskite lattice, while XPS analysis before and after OER revealed surface reconstruction with the formation of catalytically active oxyhydroxide species. Gas chromatography confirmed the highest oxygen Faradaic efficiency for P7 among all samples. Furthermore, membrane electrode assembly (MEA) testing in a zero-gap electrolyzer demonstrated efficient hydrogen production with a Faradaic efficiency of ~59% and energy efficiencies of ~44% (HHV) and ~37% (LHV). These findings demonstrate that Ni–Fe dual substitution effectively enhances the activity and durability of La00.7Sr0.3CoO3, highlighting non-equimolar high-entropy perovskites as promising OER electrocatalysts for alkaline water electrolysis.

Spin Polarized Chiral Materials for Catalytic/Asymmetric Catalytic Multicarbon CO2 Reduction

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The conversion of CO2 and inorganic small molecules into high-value-added chemicals not only deepens the scientific understanding of natural carbon cycling processes but also represents a key pathway toward achieving the "Dual Carbon" strategic goals. However, such reactions still face challenges including difficult activation, inefficient C-C, C-N, and C-O coupling, and low selectivity, urgently calling for the development of novel catalytic systems. We have pioneered two new principles: "spin-polarized intermediate stabilization via chiral structures for promoting CO2 valorization to multi-carbon products" and "spin-polarization dynamics control of asymmetric catalysis by chiral structures." These breakthroughs transcend the limitations of conventional catalysis in reaction pathway regulation, enabling efficient synthesis of multi-carbon products and highly enantioselective synthesis of chiral biomolecules.

(1) Chiral lattice-distorted inorganic materials were synthesized using chiral molecular inducers. By tuning the chiral structure to induce spin polarization effects, the electron transport mechanism was elucidated1,2. Using CO2 and water as feedstocks, photocatalytic ethanol production reached a yield of 1.4 mmol g-1 h-1 with 93.7% selectivity1, while acetic acid production achieved 0.96 mmol g-1 h-1 with 97.3% selectivity2. (2) For the first time, amino acids with enantiomeric excess (ee) > 90% were synthesized from CO2 and aqueous ammonia via photocatalysis3. It was discovered that chiral materials can lower the energy barrier for multi-carbon product formation in photocatalysis through spin polarization effects, enhance C-C, C-N, and C-O coupling efficiency, and improve overall reaction performance. A novel spin-based CO2 reduction mechanism and an enantioselective mechanism were thereby proposed.

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Sophisticated Control of Hierarchical Nanoporous Carbons for Energy Applications

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Hierarchically porous carbon materials are promising for electrochemical energy storage and conversion, but their performance depends on the accessibility of internal surfaces and the distribution of catalytically active sites. This presentation describes a template-mediated synthetic strategy for producing two-dimensional hollow turtle shell-like mesoporous carbon (HTMC), and its subsequent modification with cobalt sub-nanometre clusters.

In the first study, graphene oxide was used as a two-dimensional scaffold for the *in situ* growth of zeolitic imidazolate framework-8 (ZIF-8), followed by coating with mesostructured polydopamine. Carbonisation yielded carbon sheets with hollow macroporous chambers, mesoporous shells, and additional microporosity. Comparisons with related microporous and mesoporous carbon controls demonstrated how this hierarchical architecture mitigated restacking and improved electrochemical access to the carbon surface. As a capacitive electrode in 1 M H_2SO_4, HTMC achieved specific capacitances of 334.47 F g^{-1} at 1 mV s^{-1} and 93.7 F g^{-1} at 500 mV s^{-1}.

Building upon this architecture, the second study introduced cobalt through bimetallic cobalt–zinc ZIF precursors. Controlling the cobalt feed concentration enabled the incorporation of dispersed sub-nanometre cobalt species within nitrogen-doped carbon, while excessive cobalt feed promoted cobalt nanoparticle formation and carbon structural destruction. The resulting materials were assessed as platinum-group-metal-free electrocatalysts for the oxygen reduction reaction in alkaline electrolyte. In 0.1 M KOH, the optimum CoHTMC-1.0 material exhibited a half-wave potential of 0.786 V versus the reversible hydrogen electrode, an average electron-transfer number of 3.81, and an average hydrogen peroxide yield of 9.31%.

Together, these studies illustrate how template design and precursor-composition control can be used to tailor hierarchical nanoporous carbons for both electrochemical energy storage and electrocatalysis.

Overcoming Reductive Degradation of PTFE in High Energy Density Solvent-Free Anodes

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Dry coating is a promising approach for fabricating thick electrodes in high-energy-density lithium-ion batteries (LIBs). However, the use of polytetrafluoroethylene (PTFE) as the primary binder is limited by its intrinsic electrochemical instability at anode potentials. The low-lying lowest unoccupied molecular orbital (LUMO) of PTFE makes it susceptible to reduction, leading to low initial Coulombic efficiency

(ICE) and rapid structural degradation during cycling. To address this bottleneck, we propose a synergistic binder strategy that combines molecular engineering of PTFE with a functional co-binder. We first elevate the frontier orbital energy of the PTFE fibrous network by replacing part of the strongly electron-withdrawing fluorine with weakly electron-withdrawing oxygen- and nitrogen-containing groups through O_2 plasma treatment and gas-phase nitridation. This modification raises the LUMO energy and thereby suppresses reductive decomposition of the PTFE backbone. On this stabilized network, a co-binder is incorporated to maximize interfacial adhesion with the active materials. The dual-binder approach not only mitigates PTFE reduction but also reinforces the mechanical robustness of the three-dimensional electrode architecture against volume expansion and parasitic reactions. As a result, dry-processed anodes based on this strategy exhibit enhanced electrochemical stability, with improved ICE and long-term cycling performance accompanied by negligible microstructural degradation. Our findings demonstrate that combining frontier-orbital- engineered PTFE with a structurally reinforcing co-binder is a practical and scalable solution for robust, high-energy-density dry anodes in next-generation LIBs.

Stable In-Water Operation of Acid-Treated PEDOT:PSS Thermoelectric Films

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While PEDOT:PSS is a highly promising organic thermoelectric material, its instability in aqueous environments remains a critical limitation for practical device applications. To address this challenge, this study investigates the in-water stability and thermoelectric performance of PEDOT:PSS films post-treated with three different acids: sulfuric acid (H 2 SO 4), methanesulfonic acid (MSA), and acetic acid (AcOH). Among the acid-treated films, the H 2 SO 4 -treated films exhibited superior macroscopic and microscopic stability in water while maintaining high electrical conductivity. In contrast, the AcOH-treated and MSA-treated films underwent relatively severe structural degradation, accompanied by a substantial reduction in thickness due to the dissolution of the PSS-rich phase into water. Raman spectroscopy further revealed a blue shift of the characteristic PEDOT peaks after acid treatment, indicating a rearrangement of the polymer chains into a more structurally stable conformation favorable for maintaining conductive pathways. In particular, strong acid treatment effectively stabilized the PEDOT network, suppressing water-induced swelling, dissolution, and structural degradation. Long-term device stability tests further demonstrated that the thermoelectric generators based on H 2 SO 4 -treated films maintained stable open-circuit voltage and maximum power output during continuous underwater operation for up to 30 days. This research provides an effective strategy for developing highly durable, water-resistant organic thermoelectric materials.

Self-Healing and Recoverable Organic Thermoelectrics Enabled by Single-Walled Carbon Nanotube-Based Ternary Composites

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Organic thermoelectric materials are promising for wearable and self-powered electronics owing to their flexibility, low thermal conductivity, and solution processability. However, mechanical damage during use can disrupt conductive pathways and degrade TE performance, highlighting the need for damage-resilient materials capable of restoring their functionality for long-term operation. Herein, we report a self-healable and recoverable ternary organic composite of single-walled carbon nanotubes (SWCNTs), carboxymethyl cellulose (CMC), and Triton X-100 (TX100). Their homogeneous aqueous dispersion forms a synergistically interacting conductive network with enhanced deformability and mobility upon film formation. TX100 modulated intermolecular interactions and softened the composite network, enhancing elongation at break while reducing tensile strength. The optimized film exhibited a power factor of 46.72 μW m^{-1} K^{-2} and retained approximately 90 % of its initial value under tensile deformation. After complete cutting, the film recovered 57 % of its initial power factor through intrinsic self-healing under ambient conditions and 97 % after water-assisted recovery, with substantial restoration of electrical transport. These results demonstrate that synergistic interactions among SWCNTs, CMC, and TX100 enable the integration of robust conductive networks, mechanical deformability, and healing capability, offering a simple strategy for durable and recoverable organic thermoelectric devices.

Electronically Conductive Composite Binder for High-Performance Silicon-Based Electrodes in Lithium-Ion Batteries

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Silicon-based anodes are attractive for high-energy lithium-ion batteries (LIBs), yet their long-term operation is hindered by mechanically induced loss of electronic connectivity during repeated volume changes. Here, we report a multifunctional conductive binder that integrates electronically conductive polymer domains with functionalized carbon nanotubes to construct a resilient electron-transport network within SiO x /graphite composite electrodes.

Molecular regulation of the polymer composition enables simultaneous control over electronic conduction, dispersion stability, and mechanical cohesion, revealing that durable cycling requires a balanced combination of these properties rather than maximizing any single function. The resulting binder suppresses resistance growth and structural degradation by maintaining continuous electronic pathways under repeated electrochemical deformation. When implemented in SiO x /graphite||LiNi 0.6 Co 0.2 Mn 0.2 O 2 full cells, the optimized conductive network enables stable cycling over 1000 cycles. Notably, the electrode maintains robust operation without conventional carbon black, highlighting the potential to reduce inactive components while preserving electrical integrity. This

work establishes multifunctional polymer composite design as an effective strategy for stabilizing mechanically dynamic, high- capacity battery electrodes.

Sustainable Cherry Blossom-Based Triboelectric Nanogenerator for Self- Powered Energy Harvesting and Intelligent Human–Machine Interfaces

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The rapid development of portable and wearable electronics has created an increasing demand for sustainable, lightweight, miniaturized, and self-powered energy technologies. Triboelectric nanogenerators (TENGs), which convert ambient mechanical energy into electrical energy through contact electrification and electrostatic induction, have emerged as promising candidates for powering next-generation electronic and sensing systems. However, many high-performance TENGs rely on synthetic and non-recyclable polymeric materials, raising concerns regarding their environmental sustainability and long-term waste generation. Herein, we demonstrate a sustainable triboelectric nanogenerator utilizing naturally derived cherry blossom (CB) petals as a bio-waste dielectric layer, providing a renewable alternative to conventional synthetic triboelectric materials. The fundamental charge-transfer characteristics of the cherry blossom-based triboelectric interface were systematically investigated using experimental and theoretical approaches. Kelvin probe force microscopy (KPFM) was employed to evaluate the surface potential and verify the triboelectric polarity of the CB layer, while density functional theory (DFT) calculations were used to investigate the interfacial charge-transfer mechanism. The resulting cherry blossom-based triboelectric nanogenerator (CB-TENG) exhibited excellent electrical performance, achieving an open-circuit voltage of 613 V, a short-circuit current of 19.3 μA, and a maximum power density of 173.3 μW cm^{-2}. In addition to its high electrical output, the CB-TENG demonstrated excellent mechanical and environmental durability. The device maintained stable triboelectric performance over 22,500 repeated operating cycles, demonstrating its suitability for long-term mechanical energy harvesting. Furthermore, stable device operation was achieved over a broad temperature range from −4 °C to 100 °C, highlighting the thermal robustness of the naturally derived triboelectric layer and its potential for operation under challenging environmental conditions. The generated electrical energy was sufficient to successfully illuminate 180 commercial LEDs, demonstrating the practical energy-harvesting capability of the device. Beyond energy generation, the CB-TENG was further demonstrated as a self-powered touch-sensitive platform capable of operating under high-temperature conditions. Distinct electrical signatures generated through single- and double-tap interactions were analyzed using a Random Forest machine-learning classifier, achieving a classification accuracy of 94.74%. This integration of sustainable triboelectric energy harvesting with intelligent signal recognition demonstrates the potential of naturally derived materials for multifunctional self-powered electronics. Overall, this work establishes naturally available cherry blossom bio-waste as a promising triboelectric active material and demonstrates its potential for developing sustainable, high-output energy harvesters and self-powered human–machine interfaces. The combination of high electrical performance, mechanical durability, broad-temperature operation, and machine-learning-assisted gesture recognition provides a promising pathway toward environmentally responsible wearable and interactive electronic technologies.

Rational Design of Large-Format Sulfide-Based Solid-State Batteries for Low-Temperature Operation

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Sulfide-based solid-state batteries (SSBs) are promising for low-temperature applications owing to the favorable ionic conductivity of sulfide solid electrolytes under subzero conditions. However, their practical performance remains inferior to that of commercial lithium-ion batteries. Importantly, thermal behavior can differ substantially between lab-scale and large-format cells, highlighting the need for performance evaluation in large-format configurations. Because experimental realization of large-format SSBs remains technically challenging, we develop a stack-resolved thermo-electrochemical model that accounts for the internal cell architecture and associated thermal behavior. The model resolves individual cell components and incorporates experimentally determined electrochemical parameters together with structural parameters derived from digital-twin electrode microstructures.

Systematic analysis of cell-design parameters reveals that electrochemical performance at −32 °C is strongly governed by internal heat generation and retention. Specifically, higher electrode areal capacity promotes cell warm- up during discharge, partially offsetting the kinetic limitations under such conditions. Reducing the electrode area further enhances heat retention within the cell. Through rational design of these design parameters, the predicted performance can approach that of commercial lithium-ion batteries. This work highlights the critical interplay between electrochemical kinetics and cell-scale thermal behavior and provides practical design guidelines for large- format solid-state batteries operating under extreme low-temperature conditions.

Durable Anticorrosion Coating for Metallic Substrates

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Corrosion of metallic structures causes significant economic losses and safety risks across different industries, necessitating durable and environmentally sustainable protective coatings. Conventional anticorrosion coatings commonly rely on chromium- and lead-based additives that raise environmental and health concerns. Here, we present a nano-architectured waterborne polyurethane (WPU) coating reinforced with cellulose nanocrystals (CNCs) and functional corrosion-inhibitor nanocontainers to achieve enhanced durability and corrosion resistance. CNCs were incorporated as a

bio-derived reinforcing agent, forming a dense composite film through an extensive hydrogen-bonding network with the WPU matrix, thereby improving interfacial cohesion and mechanical robustness. Benzotriazole (BTA), an environmentally benign corrosion inhibitor, was encapsulated into zeolitic imidazolate framework-8 (ZIF-8), followed by coating with a mesoporous silica shell to form BTA-ZIF-8@mSiO 2 nanocontainers with a higher inhibitor loading. The resulting composite coating delivers dual protection. Firstly, the protection was through a mechanically strengthened physical barrier by CNCs, and secondly, through long-term corrosion inhibition via pH-responsive BTA release. Electrochemical impedance spectroscopy demonstrated an impedance modulus exceeding 10 10 Ω·cm 2 after 28 days, while pull-off testing revealed a high adhesion strength of 4.9 MPa. This work demonstrates an efficient strategy for designing high-performance anticorrosion coatings by integrating bio-based nanofillers with smart inhibitor-delivery systems.

In-Situ Electrochemical Transformation of HKUST-1 into Mixed-Valence Oxide-Derived Copper for Selective CO_2-to-C_2 + Conversion

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Copper is unique in its ability of electrochemically reducing CO 2 to multicarbon (C 2+) products, and oxide-derived copper with mixed Cu + /Cu 0 valence states is particularly effective at promoting C-C coupling for C 2+ products. On the other hand, metal-organic frameworks are attractive as high-surface-area material precursors, but they are typically converted into active forms by energy intensive processes such as pyrolysis. Our research showed that a copper MOF material (HKUST-1) can be transformed in-situ, under mild electrochemical conditions, into high-surface-area mixed-valence copper, with its resulting state dictated by the treatment environment. Although the framework is universally unstable in aqueous electrolyte, alternating the electrolyte and gas feed yields materials with surface compositions that span from Cu(OH) 2 /CuO to Cu 2 O/Cu. EPR spin-trapping revealed that in-situ hydroxyl-radical (•OH) generation, from both bicarbonate and the gas-liquid interface drives the oxide formation through a reduction-oxidation “seesaw” that sustains Cu δ^+ formation under cathodic bias. The most oxide-biased catalyst achieves ~71% C_2 + Faradaic efficiency and ~127 mA cm^{-2} partial current density toward C_2 + at −1.58 V vs RHE. The results can improve understanding of fundamental processes and lead to the establishment of a facile, low-energy route to synthesise tunable mixed-valence copper catalysts from MOFs.

Balancing Transparency and Catalytic Activity in NiFeCoO x Cocatalysts for Photoelectrochemical Water Oxidation

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Introduction: Photoelectrochemical (PEC) water splitting has attracted considerable attention as a promising approach for sustainable hydrogen production using solar energy and water. [1] High-performance PEC systems require photoelectrodes capable of efficient light absorption, efficient photogenerated charge separation, and sufficient catalytic activity. One effective strategy for enhancing PEC water splitting performance is the incorporation of cocatalysts that promote the oxygen evolution reaction (OER) while minimizing undesirable losses in optical transmittance. [2] Our group has demonstrated that semitransparent NiFeO x electrocatalysts with an optimized surface loading amount (G) enhanced OER activity while maintaining high visible-light transmittance. [2,3] These findings highlighted the importance of balancing cocatalyst coverage and light transmission in tandem-type PEC systems. [3] Herein, we investigate Co incorporation into the NiFeO x matrix to modify the electronic properties and surface reactivity of the cocatalyst. Co-based materials exhibit high intrinsic OER activity, [4] and NiFeCoO x is expected to provide synergistically enhanced catalytic performance while maintaining optical transparency. This work aims to elucidate the influence of Co incorporation on OER kinetics, optical transmittance, and interfacial stability toward the development of high-performance cocatalyst layer for semitransparent PEC photoanodes.

Experimental: NiFeCoO x precursor solutions were prepared by dissolving Ni(II)-2-ethylhexanoate, Fe(III)-2- ethylhexanoate, and Co(II)-2-ethylhexanoate in n-hexane. [2,3] A 20 mL portion of this solution was dropped onto Fe 2 O 3 thin film prepared on a fluorine-doped SnO 2 (FTO) conductive glass substrate. The coated samples were then annealed in air. The surface loading G of NiFeCoO x on Fe 2 O 3 /FTO electrode was precisely controlled in the range of 0.02–1.0 mmol cm -2 by varying the precursor concentration. PEC measurements were performed using three- electrode configuration, with NiFeCoO x /Fe 2 O 3 /FTO photoelectrode, a coiled Pt wire counter electrode, Ag/AgCl sat'd KCl reference electrode. All measurements were conducted in 1.0 M KOH aqueous solution under an Ar atmosphere. Simulated solar illumination (AM 1.5G, 100 mW cm -2) was used as the light source. Photoelectrode potentials were converted to the potential of reversible hydrogen electrode (V RHE) scale. Results and Discussion: NiFeCoO x /Fe 2 O 3 /FTO with a G of 0.20 mmol cm -2 exhibited the highest PEC OER activity. The onset potentials for Fe 2 O 3 photoanodes modified with NiFeCoO x and NiFeO x were found to be 0.52 V RHE and 0.65 V RHE , respectively, indicating that the addition of Co improves PEC OER performance, specifically due to the lower OER overpotential of NiFeCoO x . The NiFeCoO x /Fe 2 O 3 /FTO photoanode produced a photocurrent density of 0.14 mA cm -2 at 1.23 V RHE , which is approximately twice that of NiFeO x /Fe 2 O 3 /FTO. At the optimal loading, the NiFeCoO x layer maintained high optical transparency without significantly hindering light absorption by the Fe 2 O 3 photoanode. Thus, NiFeCoO x offers a promising ternary cocatalyst design for PEC applications, combining transparency and high activity more effectively than the binary NiFeO x cocatalyst.

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Session: Ceramics, Polymers and Composite Materials

From polymer grafting to messenger materials and sustainable metamaterials

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Polymer surface modification offers unique possibilities for creating interactive and functional materials. Polymer grafting in particular can be employed for nanoscale control both on macroscopic surfaces and for nanoparticles and I will discuss the implications for self-reporting surfaces and metamaterials.

Polymer brush surfaces that alter their physical properties in response to chemical stimuli have the capacity to be used as so-called Messenger materials. These materials translate local physicochemical changes into spatially-resolved modulation of fluorescence [1]. This approach can be used for unraveling contact mechanics and friction in complex scenarios as well as clarify mechanisms acting in responsive and adaptive surface coatings.

Polymer modification of nanoparticles results in hairy nanoparticles, which find a range of applications in functional materials [2]. Especially metallic nanoparticles offer a number of interesting optical and electronic effects due to their localized surface plasmon resonance (LSPR) Adding a functional polymeric shell does not only allow controlling inter-particle distances but as well tailor transport / electronic couping. [2,3] Increasing the level of complexity, the ordering of particles at different length scales opens another powerful route to optical and electronic functionality due to novel collective plasmonic excitations arising from plasmonic coupling effects. We focus on achieving such ordered particle arrays through self-assembly approaches. Colloidal self-assembly can indeed yield well-defined colloidal clusters and surface arrays in which coupling effects can be controlled. In particular, large-scale assemblies are possible in combination with biomimetic surface patterning like controlled wrinkling. We discuss the underlying physicochemical principles of the structure formation process and the resulting plasmonic coupling effects including chiroplasmonic metamaterial effects [4,5]. Finally, we present perspectives on how these assembly principles can be relevant for developing circular economy approaches for advanced materials.

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All-Dislocation-Ceramics for High Ionic Conductivity and High Fracture Toughness; Possible Production by Cold Sintering

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Conventional lithium-ion batteries have a safety problem that they are burnable upon heating by vaporization of the organic solvents. In order to solve the safety problem, all-solid-state batteries have been studied because they are not burnable. However, ionic conductivity of many solid electrolytes is considerably lower than that of liquid electrolytes. In order to improve the ionic conductivity of solid electrolytes, the authors have suggested all- dislocation-ceramics which are solid electrolytes filled with appropriate dislocation-pipes [1, 2]. Due to the high vacancy concentration around a dislocation and the reduction of the energy barrier for ionic conduction by the strain field of a dislocation, ionic conductivity along a dislocation could be several orders of magnitude higher than that in the bulk [1, 3]. Furthermore, as the solid electrolytes are filled with appropriate dislocation-pipes, ionic current density is nearly spatially uniform and dendrite formation could be avoided [4]. Fracture toughness could also be increased by the presence of dislocations, resulting in the absence of dendrite formation [1, 2]. In the present study, evolution of mobile and immobile dislocations inside solid electrolytes during cold sintering under applied pressure is numerically simulated [5]. Cold sintering is sintering with the aid of liquid phase such as water usually under applied pressure. The results indicate that all-dislocation-ceramics could be produced during cold sintering process if the solid electrolytes are relatively ductile. Experimental studies are required on the fabrication of all-dislocation- ceramics by cold sintering.

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Defect Engineering in Oxides via Flash Sintering

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In ceramics, defects are crucial in facilitating transport, stabilizing structures, and tuning optical absorption properties. Through the injection of oxygen vacancies, DC flash sintering is widely accepted to drive electrochemical blackening of yttria-stabilized zirconia (YSZ). Furthermore, point and extended defects are viewed by the community not merely by-products of the flash event but are central to both its ignition and its outcomes.

While flash sintering has been established as a promising technology to rapidly densify ceramics with externally applied electrical field or current, the capability of engineering defects with flash sintering in ceramics to control their physical properties has not been fully explored. Through deliberate manipulation of defect chemistry (oxygen non-stoichiometry, doping), it is possible to lower the onset temperature and to tune the properties of flash-sintered materials. In this talk, we present our mechanistic inspection of flash sintering onset of YSZ through electrochemical impedance spectroscopy. In addition, we will discuss the optimization process of defect engineered ZnO composite in enhancing its photocatalysis performance for toxic chemicals removal from environmental waters.

Advanced Processing and Fatigue Behavior of Carbon Nanotube Reinforced Aluminum Matrix Hybrid Composites

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Aluminum matrix composites reinforced with carbon nanotubes (CNTs) have attracted considerable interest as next-generation lightweight structural materials due to their exceptional potential for achieving high strength-to-weight ratios. The outstanding mechanical properties of CNTs, including high tensile strength, stiffness, and low density, offer significant advantages when incorporated into metallic matrices. However, challenges such as CNT agglomeration, weak interfacial bonding, and structural damage during processing must be addressed to fully exploit their reinforcing capabilities.

In this study, CNT/Al composites were developed through a carefully designed multi-step processing route aimed at achieving uniform CNT dispersion and strong interfacial bonding. CNTs were first

dispersed in the aluminum matrix using a combination of chemical and mechanical treatments, including ultrasonic agitation in an organic solvent, N,N-Dimethylethanamide (DMAc), with potassium carbonate (K_2CO_3) as a dispersant. This chemical dispersion step was followed by dry ball milling to further distribute CNTs within the aluminum powder. The composite powders were then consolidated using spark plasma sintering (SPS), which enabled rapid densification while minimizing grain growth and CNT degradation. A post-SPS hot-rolling treatment was subsequently applied to refine the microstructure, improve densification, and enhance CNT alignment and interfacial bonding. Mechanical performance was evaluated through tensile testing, Vickers hardness measurements, and tension-compression low-cycle fatigue tests. Microstructural characterization using SEM and TEM provided insights into CNT dispersion, grain refinement, and interfacial features. The results demonstrated that CNT addition significantly increased the yield strength and ultimate tensile strength of the aluminum matrix through load-transfer strengthening, grain refinement, and dislocation-based mechanisms. Fractographic analysis of fatigue-tested samples revealed that CNTs effectively suppressed crack initiation and growth, contributing to improved fatigue resistance.

A notable finding was the pronounced influence of CNTs on the Bauschinger effect. The presence of CNTs increased back stresses within the aluminum matrix, thereby enhancing the Bauschinger effect. Interestingly, an increase in the Bauschinger effect was correlated with longer tension-compression low-cycle fatigue life, suggesting that CNT-induced internal stress redistribution plays a beneficial role in cyclic deformation behavior. Post-SPS hot rolling further improved fatigue life by strengthening CNT-Al interfacial bonding and reducing residual porosity. Beyond monolithic CNT/Al composites, hybrid composites incorporating TiC, TiB_2, and $BaTiO_3$ were also developed. TiC and TiB_2 additions led to simultaneous improvements in tensile strength, ductility, and fatigue resistance due to synergistic strengthening mechanisms. In contrast, $BaTiO_3$-containing composites exhibited electromechanical responses during fatigue loading, enabling health-monitoring functionality. Their fatigue behavior, influenced by the Bauschinger effect, was reflected in measurable changes in electric potential difference and analyzed using a one-dimensional micromechanical model. Overall, this study highlights the importance of optimized CNT dispersion, interfacial engineering, and hybrid reinforcement strategies for achieving high-performance CNT/Al composites suitable for lightweight structural and multifunctional applications.

Why Do Strong Carbon Nanotube Yarns Produce Weak Composites?

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Carbon nanotube (CNT) yarns have emerged as promising reinforcement materials for next-generation lightweight structural composites because of their outstanding tensile properties and low density. Recent advances in CNT synthesis and yarn fabrication have enabled tensile strengths approaching, and in some cases exceeding, those of conventional high-performance carbon fibers. Surprisingly, however, embedding CNT yarns into polymer matrices often results in composite strengths far below those anticipated from the constituent yarn properties. This apparent contradiction suggests that simply improving the intrinsic strength of CNT yarns is insufficient for realizing high-performance structural composites. Instead, a fundamental understanding of how hierarchical CNT yarns transfer load and accumulate damage within polymer matrices is required. We hypothesize that the mechanical behavior of CNT-yarn composites cannot be adequately interpreted using the failure

concepts established for conventional brittle-fiber-reinforced composites. To examine this hypothesis, the damage evolution and load-transfer behavior of epoxy-embedded CNT yarns were investigated using a multiscale characterization approach integrating synchrotron radiation X-ray computed tomography (SRXCT), digital volume correlation (DVC), Raman spectroscopy, and high-resolution nano-computed tomography (nano-CT). These complementary techniques enabled simultaneous observation of internal damage, three-dimensional matrix strain fields, local stress transfer within the yarn, and nanoscale structural changes that could not be resolved using conventional X-ray CT alone. The results were compared with those obtained from carbon-fiber-reinforced composites to clarify the influence of the hierarchical architecture unique to CNT yarns. The experiments consistently revealed that damage evolution in CNT-yarn composites differs fundamentally from that in conventional carbon-fiber composites. Instead of localized fiber fracture followed by stress recovery, tensile loading induced gradual deterioration of load transfer through spatially distributed inter- bundle damage. DVC identified heterogeneous strain fields within the surrounding epoxy matrix, while Raman spectroscopy demonstrated highly non-uniform axial strain distributions and persistent load-bearing capability even after damage initiation. Nano-CT further revealed interfacial gaps and internal voids within regions that appeared undamaged in lower-resolution observations, indicating that sub-resolution damage was broadly distributed throughout the yarn. These observations demonstrate that local damage does not immediately eliminate the load-carrying capacity of the yarn; rather, progressive degradation of mechanical interactions among neighboring CNT bundles governs the overall tensile response.

These findings provide a new perspective on the mechanical design of hierarchical fibrous composites. The dominant mechanism controlling tensile failure is not the formation of a single critical fracture but the cumulative degradation of inter-bundle load transfer distributed throughout the yarn structure. Consequently, design methodologies derived from classical fragmentation and stress-recovery theories for brittle fibers may not be directly applicable to CNT-yarn composites. Instead, future structural design should explicitly account for hierarchical damage accumulation and progressive load-transfer degradation. This mechanistic framework offers new guidance for optimizing yarn architecture, interface design, and matrix interactions, thereby providing a foundation for the development of high-strength CNT-yarn-reinforced composite materials.

Shaping macroscopic dynamic wetting through multiscale interfacial heterogeneity

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Wetting of water on solid surfaces is ubiquitous in everyday life and plays a central role in natural and industrial processes. Contact angle hysteresis, commonly quantified by the difference between advancing and receding contact angles, is a fundamental characteristic of wetting on real solid surfaces. Low- hysteresis surfaces are highly desirable in many applications where facile droplet motion and efficient liquid removal are essential. This requirement is particularly challenging for hydrophilic surfaces, because strong water–surface affinity tends to make the contact line more sensitive to local variations in surface chemistry and structure. Such chemical and topological heterogeneity can induce contact-line pinning and is widely recognized as a major origin of contact angle hysteresis. However, how heterogeneity at molecular to nanoscale length scales governs macroscopic wetting hysteresis remains complex and insufficiently understood. In this talk, I will discuss how multiscale interfacial heterogeneity in wettability affects macroscopic wetting states and water mobility, with a focus on hydrophilic low-hysteresis surfaces. Molecularly mixed self-assembled monolayers provide an ideal platform for controlled surface design, enabling systematic investigation of how molecular-scale composition influences dynamic wetting. In contrast, hybrid polymer coatings based on complex waterborne paints offer a practical route to scalable surfaces, where hydrophilic and relatively hydrophobic polymer nanoparticles create heterogeneous wettability over tens to hundreds of nanometers. By connecting these model and practical systems, I will highlight the emergence of hydrophilic slippery behavior, in which water droplets remain highly mobile even on intrinsically hydrophilic surfaces. This counterintuitive wetting state challenges the conventional trade-off between water affinity and droplet mobility, and provides a basis for designing water-attracting yet mobile interfaces for sustainable heat and water management.

Session: Computational Materials

Investigating contact-limited scaling in sub-15-nm TMD FETs from first-principles

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Two-dimensional (2D) transition metal dichalcogenide (TMD) field-effect transistors (FETs) are promising candidates for future three-dimensional complementary metal-oxide-semiconductor (CMOS) technologies because of their distinctive physical properties, including atomically thin bodies, suitable bandgaps, and carrier mobility that can be maintained even at the ultrathin-body limit. However, the contact behavior of short-channel TMD FETs with channel lengths below 15 nm remains largely unexplored, primarily because of the stringent fabrication challenges and process limitations associated with device scaling. Here, we present a first-principles FETs contact study based on density functional theory and the non-equilibrium Green's function method. We estimate device performance for three TMD channel materials (WSe 2 , WS 2 , and MoS 2), including metal contacts (Ni) at source and drain for the first time. The results show that the variation in R c has less impact on I ON and I OFF at a given V DD than the variation in subthreshold swing (SS; with differences exceeding 30 mV/dec), suggesting SS may be more sensitive to the contacting material choice than previously realized at gate lengths below 15 nm. Among the channel and contact material combinations studied, Ni/WSe 2 FET leads to the best short-channel device performance. The quantum transport calculation shows the highest density of charge accumulation at the Ni/WSe 2 contact edge. Inspired by this first-principles study, we performed X-ray photoelectron spectroscopy and verified the bonding strength at the Ni/WSe 2 contact to be stronger than Ni/WS 2 and Ni/MoS 2 contacts. This supports the theoretical finding that the contact/channel materials need to be chosen to optimize SS and I ON in short-channel TMD FETs.

New Understanding of Sintering and Re-dispersion of Supported Nanocatalysts

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Sintering and re-dispersion are crucial for regulating the size and properties of supported nanocatalysts. Conventional theory suggests the atomically dispersed nanocatalysts are intrinsically unstable and prone to sinter to reduce surface energies. Herein, we developed a generalized thermodynamics framework to demonstrates that the nanocatalysts are prone to self-dispersion into atomic clusters by entropy effect below the critical concentration, which is further supported by machine-learning-assisted molecular dynamics simulations, in situ Cs-corrected environmental scanning transmission electron microscopy and synchrotron-based ambient pressure X-ray photoelectron spectroscopy experiments. Further we reveal an unexpected phenomenon that the

supported nanoparticles redisperse upon heating and reversibly sinter upon cooling, contrary to the traditional understanding that "high temperature promotes sintering". This theory redefines the basic understanding of the sintering, dispersion, and coexistence behavior between nanoparticles and atomically dispersed catalysts, thereby offering new strategies to tune the states of supported nanocatalysts.

From First-principles Calculations to Interpretable AI for the Rational Design of Electrochemical Energy Materials

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The rational design of nanomaterials for electrochemical energy conversion and storage is limited far less by our grasp of the underlying physics than by the size of the space in which that physics must be evaluated. A multimetallic single-atom catalyst drawn from a 27-element chemical space on a pyridinic-N_4 support already spans 10^5–10^6 distinct active-site environments, while a single density functional theory (DFT) relaxation coststhousands of CPU-hours. Machine learning is the obvious response, yet a purely data-driven surrogate carries two liabilities that matter acutely in electrocatalysis: it extrapolates unreliably beyond its training distribution, and it gives no mechanistic account of its predictions. A third constraint is the fidelity of the structural input itself — our atomic-resolution imaging of individual ligand-protected nanocrystals in solution showed that nominally identical particles differ measurably in strain field, facet occupancy and ligand coverage, so the ensemble average is a poor training target.

This presentation describes a framework combining quantum-mechanical calculations, equivariant graph neural networks, active learning and physics-informed neural potentials so that each liability is addressed by construction rather than by post-hoc correction. A site-resolved binding-energy surrogate for multimetallic single-atom catalysts toward the oxygen evolution reaction is built by training a PaiNN-based network under combined multi-task, multi- fidelity and transfer learning: the mean absolute error against DFT falls from 1.38 eV for a zero-shot universal potential to 0.38 eV (R^2 = 0.93) using only five percent of the DFT labels. Applied across the space it quantifies the cocktail effect pair-by-pair, shows six metals own ~90 % of the active tail (a ~0.3 V penalty once excluded), and reveals vanadium is unfavourable alone yet promotes activity when cobalt is dominant.

An acquisition function balancing predicted uncertainty, structural diversity and Bayesian optimization then turns the same surrogate into a self-driving campaign: over fifteen iterations the hit ratio for top-percentile active sites rises from roughly five to nearly fifty percent — equivalent coverage at a sixfold reduction in DFT calls — and two further iterations reach over 30,000 ternary sites. Finally, P^2Net, a pairwise-decomposed physics-informed network embedding an analytical bond-order-potential layer, restores extrapolation and interpretability: trained on fifty structures per system it tracks DFT far outside its training window, stays molecular-dynamics stable for 50 ps on Water-1k where the baseline fails after 1.7 ps, and predicts the S_n2 activation energy to 5.9 meV and the transition state to 0.006 Å with no transition-state training data. Together these outline a scalable, data-efficient paradigm in

which quantum mechanics supplies the ground truth, machine learning the reach, and embedded physics the transparency a design rule requires.

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Constraint-Guided Diffusion Models for Inorganic Crystal Structure Discovery

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The discovery of inorganic crystal structures with targeted properties remains a major challenge in materials science, particularly for energy-related applications such as hydrogen storage and hydrogen production. While high-throughput first-principles calculations and machine learning can efficiently screen large chemical spaces, they remain essentially limited to exploring structures that have already been proposed. Generative artificial intelligence offers a complementary approach by directly proposing new crystal structures, opening access to unexplored regions of materials space. Among generative approaches, diffusion models have recently emerged as a powerful framework for crystal structure generation. However, generating physically plausible structures is not sufficient for materials discovery. Candidate structures must simultaneously satisfy multiple constraints related to chemical composition, local atomic environments, interatomic distances, crystallographic symmetry, and ultimately thermodynamic stability.

Incorporating these requirements directly into the generation process is therefore a key challenge for reliable inverse materials design. In this work, we develop a generative framework based on diffusion models with adaptive constraint guidance. Instead of generating structures independently of physical requirements and filtering them afterwards, user-defined constraints are directly incorporated during the denoising process. This enables the generation trajectory to be guided towards chemically and

geometrically feasible configurations while retaining the stochastic nature of the generative model. Constraints can be explicitly defined according to the targeted material class, providing an interpretable mechanism for steering the exploration of crystal structure space. We apply this approach to the generation of inorganic materials mainly based on transition metals, with particular interest in compounds containing additional s–p elements under coordination constraints. The generated structures are subsequently evaluated through a multi-level validation workflow combining structural analysis by symmetrization, deduplication to retain unique phases, energy estimation using machine-learning interatomic potentials, and convex- hull analysis to assess their thermodynamic stability.

This constrained generative strategy aims to move beyond the generation of statistically plausible crystals towards the targeted exploration of physically meaningful and potentially synthesizable materials. More broadly, it provides a flexible framework in which domain knowledge and explicit physical constraints can be integrated directly into generative AI, offering a practical route toward interpretable and physics-guided inverse materials design.

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First-Principles Investigation of Hydride-Ion Transport and Ion-Exchange Mechanisms in Mixed-Anion Oxyhydrides

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Mixed-anion oxyhydrides have attracted considerable attention as a new class of functional ionics materials because they exhibit unique hydride-ion (H −) transport and redox properties that are inaccessible in conventional oxides. Our research group has pioneered the synthesis of novel oxyhydrides and aims to establish next-generation electrochemical devices, including solid electrolytes, batteries, fuel cells, and material-conversion systems, by exploiting H − conduction and the H − /H 2 redox reaction. To accelerate materials design for these applications, it is essential to understand the microscopic mechanisms governing hydride-ion transport, ion-exchange reactions, and phase stability. In this study, we employ first-principles calculations to investigate these fundamental processes from both dynamic and thermodynamic perspectives using two representative oxyhydride systems: the K 2 NiF 4 -type hydride-ion conductor Ba 1.75 LiH 2.7 O 0.9 (BLHO) and the perovskite-type mixed (electron + ion) conductor BaTiO 3−x H x (BTOH).

For the ionic conductor BLHO, first-principles molecular dynamics simulations were performed based on experimentally determined crystal structures. The calculated hydride diffusion coefficients are consistent with quasi- elastic neutron scattering (QENS) measurements, while the activation energy obtained from diffusion does not fully explain the experimentally observed ionic conductivity, indicating that long-range conductivity is governed by processes beyond simple in-plane diffusion. Analysis of the Lindemann index further reveals that the hydride sublattice undergoes disordering above the superionic transition temperature, providing strong evidence that BLHO exhibits sublattice melting, a characteristic feature of conventional superionic conductors. The collective motion of hydride ions is discussed to clarify the microscopic origin of the exceptionally high ionic conductivity.

To understand hydride incorporation and stability in perovskite BTOH, phase-diagram calculations and migration barrier analyses were carried out. Although heavily hydrogenated compositions are thermodynamically metastable, the calculations explain the experimentally observed hydrogen solubility limits by considering reaction equilibria involving CaH 2 and the CaO byproduct during topochemical synthesis. Furthermore, kinetic analysis identifies oxide-ion diffusion as the rate-limiting process during O 2− /H − ion exchange, yielding reaction times consistent with experimentally reported synthesis durations. At higher hydride concentrations, hydride diffusion becomes increasingly important, suggesting a different kinetic regime relevant to mechanochemical synthesis and isotope-exchange reactions. Together, these results provide a unified atomistic understanding of hydride-ion incorporation, transport, and phase stability in representative oxyhydrides. The combination of thermodynamic, kinetic, and dynamical analyses establishes a first-principles framework for rational design of next-generation hydride-based functional materials and electrochemical devices.

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Localized Electrochemical Imaging and Active-Site Analysis by Scanning Electrochemical Cell Microscopy

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In electrochemical energy devices, solid-liquid interfaces are intrinsically heterogeneous because their local electrochemical activity is governed by surface structure, crystal orientation, defects, composition, and ion transport pathways. Conventional electrochemical measurements average these contributions over the entire electrode and therefore obscure the specific sites that initiate or control a reaction. Scanning electrochemical cell microscopy (SECCM) overcomes this limitation by using the meniscus formed at the end of a nanopipette as a microscopic electrochemical cell. Local voltammograms are collected at independently addressed positions and assembled into electrochemical images that reveal spatial variations in reactivity [1,2].

In this talk, we summarize our recent progress in developing SECCM as a versatile platform for localized interface analysis across electrocatalysts, battery electrodes, and other electrochemical devices. The electrochemical imaging has enabled the identification of active sites for electrochemical reactions and the direct correlation of activity with local structural features. For graphene-/graphite-based electrochemical device systems, SECCM measurements revealed enhanced electrochemical activity at deliberately engineered edge [3] and dopant structures [4], demonstrating that electrocatalytic performance can be controlled through atomic-/nano-scale structural design. Related measurements on two-dimensional materials have further shown that electrochemical activity is not uniformly distributed but is concentrated at particular edges, defects, or dielectric property [5-7].

SECCM has also been extended to photoelectrochemical interfaces. Local measurements of electrochemical hydrogen evolution reveal reaction heterogeneity that cannot be resolved by conventional bulk voltammetry, while spatially resolved photocurrent measurements clarify how crystallographic and interfacial variations govern photoelectrochemical responses [8,9]. More recently, we integrated SECCM with Raman spectroscopy to simultaneously acquire localized electrochemical and structural information under operating conditions. Using single-crystalline $LiFePO_4$ as a model battery electrode, reversible lithium extraction and insertion were confined within the SECCM meniscus and accompanied by operando Raman detection of the corresponding local structural transformation [10].

The SECCM analysis is a simply and powerful mapping technique, but as an experimental framework for locating electrochemical active sites, determining their structural origins, and following their evolution during a reaction. The combined electrochemical, optical, and spectroscopic capabilities provide a route toward mechanistic understanding and rational design of functional interfaces for batteries, electrocatalysis, and photoelectrochemistry.

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Growth of Semiconductors on Insulating Crystalline Substrates

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Semiconductor films on insulating materials have application fields where high resistance to radiation is required. Applications of these material systems to opto-electrical devices or ferroelectric devices are also interesting. To achieve high performance as electronic device, quality of the semiconductor film is important. A successful example is Si on sapphire (SOS). It is known that a (100)-oriented Si grows on an r-plane sapphire. The in-plane directions also align to specific axes of the substrate. Due to the distinct orientation, the Si on r-plane sapphire is a suitable platform for radiation-resistant semiconductor devices. On the other hand, we found that a Ge film grown by MBE on a r-plane sapphire is (111)-oriented [1]. This difference despite the same crystal structure indicated an unknown

factor which determines the epitaxial relationship between sapphire and group-IV semiconductor films. We carried out an analysis based on the O-lattice theory [2] and found that the degree of lattice matching evaluated by the O- lattice theory qualitatively agreed with the experimental results [1].

This study investigates the orientation of MBE-grown group-IV films on single-crystalline quartz substrates. The crystallographic orientations of the films were analyzed using XRD pole figure measurements. We found that (100)- oriented Si grows on m-plane quartz by MBE method. This material system can be utilized as a low-cost alternative to SOS. The lower dielectric constant compared to that of sapphire is another favorable feature for high frequency applications. On the other hand, the quality of Ge grown on m-plane quartz was low. The diffraction pattern in the pole figure is obscure. The computational result obtained by the O-lattice theory shows that the degree of the lattice matching between a (100)-oriented SiGe film and a quartz substrate decreases with the Ge composition. These results indicate the importance of the lattice matching to obtain high-quality SiGe films on insulating single crystalline substrates by MBE.

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Morphological-Based Descriptions of Ferrite Formation During Nucleation.

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This presentation explores the possible effects of the nuclei morphology during the evolution of the compositions for ferritic steels. It aims to develop a statistical morphological-based model of ferritic phase transformation in hypoeutectoid steel. Most descriptions of the nuclei are usually spherical based assumptions, rare or no cases exist where other morphological assumptions have been employed and their effects studied during nucleation of ferrite. Aside the interfacial energy, some of the variable parameters like the number of sides of the shape and the shape angle, plays reasonable roles during the composition evolution and the interactions between the compositions. The approximation of the evolution of the nuclei composition, is the main interest, while the exploration of the impact of the precipitate morphology is also included. In addition, the effect of the morphology on some of the nucleation parameters like the incubation time, probability barrier and on the rate of nucleation will be highlighted.

Session: Porous Materials

Coupling Mesoporosity and Amorphous Disorder in High-Entropy Alloy Films Toward Highly Efficient Methanol Electrocatalysis

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Mesoporous high-entropy alloys (HEAs) offer a powerful platform for electrocatalysis by combining multicomponent electronic interactions with high surface accessibility. However, the low-temperature synthesis of mesoporous HEA thin films with amorphous atomic structures remains a major challenge because multielement co- reduction, entropy formation, and nanoscale porosity must be controlled simultaneously. Here, we report a potential- guided micelle-assisted electrodeposition strategy for constructing mesoporous amorphous PtPdRhCuTe HEA thin films. Block-copolymer micelles serve as pore-directing templates, while the applied deposition potential regulates multielement incorporation, configurational entropy, and crystallinity. Under the optimized deposition potential of −0.2 V, a uniform mesoporous amorphous HEA film is obtained with a well-defined porous architecture, homogeneous distribution of Pt, Pd, Rh, Cu, and Te, high configurational entropy, and an amorphous-dominant atomic arrangement. The resulting catalyst integrates three key design features: accessible mesoporous channels for efficient mass transport, high-entropy multicomponent chemistry for electronic modulation, and amorphous disorder for generating diverse active sites. As a result, the mesoporous amorphous PtPdRhCuTe HEA film exhibits superior performance in methanol oxidation reaction, with a specific activity of 2.39 mA cm –2 and a mass activity of 0.67 A mg –1 , outperforming both the crystalline HEA counterpart and commercial Pt/C. This work establishes potential- guided electrodeposition as a versatile route for designing mesoporous amorphous multicomponent alloy films and provides a new materials platform for high-performance electrocatalysis.

Keywords: mesoporous, amorphous, high-entropy alloy, low-temperature synthesis.

Synthesis of Single-Crystalline Ordered Nanoporous Metal Oxides by Confined Crystal Growth inside Silica Colloidal Crystals

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Hard-templating method is a versatile approach for constructing ordered nanoporous metal oxides. Pore walls of nanoporous metal oxides generally consist of aggregates of small crystallites, and their pore walls therefore contain numerous grain boundaries. Because grain boundaries strongly affect carrier transport, structural stability, and other functional properties, controlling crystal growth while preserving an ordered nanoporous structure is an important challenge in the synthesis of nanoporous metal oxides. 1 Recently, we have developed a chemical-vapor-based confined crystal-growth (C 3) method for preparing single-crystalline ordered nanoporous metal oxides using silica colloidal crystals as hard templates. 2 In this method, metal chlorides are introduced into the interstitial nanopores of the silica template and converted into metal oxides by reaction with oxygen during heating. Unlike commonly used nitrate, acetate, and alkoxide precursors, metal chlorides do not directly generate oxide nuclei through thermal decomposition. They are transported through the confined pore space in the vapor phase and react with oxygen supplied from outside the template. Continuous supply of the precursor within the template enables crystal growth while suppressing excessive nucleation, allowing the formation of nanoporous metal oxides with substantially enlarged crystallite sizes.

The applicability of this strategy has been demonstrated for α-Fe 2 O 3 2 and indium tin oxide (ITO) 3,4 . The resulting nanoporous α-Fe 2 O 3 possesses spherical pores of approximately 54 nm, reflecting the arrangement of the template silica nanospheres, while individual crystalline domains extend from several hundred nanometers to several micrometers. Compared with conventional nanoporous α-Fe 2 O 3 composed of small crystallites, the single-crystalline material retains its ordered porous structure even after high-temperature treatment. It also exhibits high activity for methylene blue degradation through the photo-Fenton reaction, which is attributed to suppressed recombination of photogenerated electrons and holes resulting from the reduced number of grain boundaries.

Simultaneously achieving high carrier conductivity and low thermal conductivity is an important requirement for thermoelectric materials, and single-crystalline nanoporous ITO further demonstrates the potential of this structural design for controlling transport properties. The material exhibits relatively high electrical conductivity compared with conventional nanoporous ITO composed of small crystallites while maintaining the low thermal conductivity associated with its nanoporous architecture. These results demonstrate that controlling crystal growth within a preorganized nanospace provides a route to combining ordered porosity with high crystallinity and enables the design of nanoporous oxides in which structural and transport properties can be tailored.

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Ultrasonic Monitoring of Zeolite and MOF Crystallization

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The investigation and understanding of the underlying mechanisms for the crystallization of molecular sieve materials such as metal-organic frameworks (MOFs) and zeolites have received increasing interest in recent years. This is mainly because improvements of the corresponding equipment were made that is essential for in situ diagnostics. In contrast to classical techniques, such as X-ray diffraction and neutron scattering, nuclear magnetic resonance or infrared and Raman spectroscopy, ultrasonic monitoring has not received proper attention [1]. Thereby, especially for zeolites, important insights have been gained with this technique already. In the present study, we report the successful use of ultrasonic device as a real-time, in- situ diagnostic tool for monitoring the crystallization progress of zeolite A from homogeneous, colloidal solution. Kinetic information like reaction rate or reaction order of crystal growth can easily be calculated from the measured ultrasonic signal data. For the mathematicaldescription of the crystallization curves, the experimental curves were fitted with different kinetic models [2]. The crystallization proceeds in more than one step suggesting a change of the kinetics during the formation of the crystalline material. The understanding of metal organic framework syntheses is still a challenging task in the field of porous materials. Proposed models for the MOF formation mechanisms includes the formation of pre- nucleation building units (PNBU), which are “the minimum assembly of atoms, ions or molecules which, by condensation of the group with others (identical or different) give rise to the final solid” [2]. The nature of these PNBUs is widely discussed, but detailed insights are still rare. In this study, ZIF-8 with varying particle size and morphology is synthesized from zinc nitrate hexahydrate, 2- methylimidazole and CTAB in different solvents. In our study, we found that the ultrasonic attenuation already increases rapidly within the first minute of the ZIF-8 syntheses. Depending on the molar ratio of linker to metal and the water content, not only the final particle size, but also the course of the ultrasonic signal changes [4].

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Comparison of four types of alumina adsorbents developed for domestic production of 99 Mo/ 99m Tc

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Objective

Japan relies entirely on imports for molybdenum-99 (99 Mo), the parent nuclide of technetium-99m (99m Tc), which is frequently used in nuclear medicine diagnostic procedures. This total dependence poses a significant challenge for a stable supply. A promising solution is the domestic production of 99 Mo through the activation of natural Mo, followed by the extraction of 99m Tc via a generator. However, this method requires a Mo adsorption capacity exceeeding 200 mg/g, which is unattainable with conventional alumina (2–10 mg/g). In this study, we compared the Mo adsorption capacities of four types of alumina adsorbents developed to overcome this limitation.

Methods

We have conducted research and development on four distinct types of alumina adsorbents:

1. Mesoporous silica-alumina composite
2. Solvothermal-derived alumina
3. Titanium-doped alumina
4. Spray-dried alumina

The adsorption performance of these four materials was evaluated and compared.

Results

 Mesoporous silica-alumina composite: The adsorption capacity depended on the calcination temperature, pH, and precursor mixing molecular weight ratio, reaching a maximum Mo adsorption capacity of 16.2 mg/g.

 Solvothermal-derived alumina: The capacity was influenced by the calcination temperature and precursor mixing molecular weight ratio, with a maximum capacity of 56.2 mg/g.

 Titanium-doped alumina: The capacity depended on the precursor mixing molecular weight ratio, achieving a maximum of 44.5 mg/g.

 Spray-drying method: The capacity varied according to the separation method and calcination temperature. The extracted sample exhibited the highest maximum Mo adsorption capacity of 82.6 mg/g.

Conclusion

In conclusion, the spray-drying method (after extraction) yielded the highest Mo adsorption capacity of 82.6 mg/g among the four types of alumina adsorbents developed to facilitate the domestic production of radioisotopes. This superior performance is primarily attributed to the preservation of a high density of surface hydroxyl groups. By bypassing the high-temperature calcination process, the reduction of active adsorption sites that typically occurs in conventional materials was minimised. While this achievement marks a significant technical advancement over the limited capacity of standard alumina (2–10 mg/g), the current value remains below the 200 mg/g threshold required for the practical implementation of generator systems using natural molybdenum. Future research will prioritize the refinement of the spray-drying synthesis and the optimization of pore structures to further enhance adsorption efficiency. These developments are essential for bridging the performance gap and ultimately securing a stable, autonomous supply of medical radioisotopes for nuclear medicine in Japan.

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

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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, cost-effective hydrogen production that contributes to the transition to clean energy.

Metal-Organic Framework-Templated Deconstruction-Reconstruction Enables One- Dimensional to Two-Dimensional Self-Assembly of Nickel Phosphates for High-Performance Ammonia Sensing

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Self-assembled nanomaterials formed through the spontaneous organisation of nanoscale building blocks are attractive because of their high surface areas, strong interparticle connectivity, and ease of processing. However, programming the assembly of one-dimensional (1D) transition-metal nanostructures into two-dimensional (2D) architectures remains challenging because of dimensional mismatch and kinetic or thermodynamic barriers. Here, we report a general metal-organic framework (MOF)-templating strategy that enables the 1D-to-2D self-assembly of nickel phosphate into nanofibre-assembled quasi-nanosheets (QNSs). The conversion proceeds through an acid- driven deconstruction-reconstruction (ADR) mechanism, in which Ni-MOFs act as dissolution-programmable metal reservoirs that regulate local Ni 2+ release and phosphate nucleation. This process first generates nickel phosphate nanofibres and subsequently drives their secondary assembly into QNSs. By varying the Ni-MOF linker chemistry, the porosity and specific surface area of the resulting QNSs

can be readily tuned, and the strategy can be extended to bimetallic phosphate analogues. As a proof-of-concept sensing platform, the Ni-BPDC-derived QNSs exhibit a high response to ammonia (NH 3), with a frequency shift of 897.9 ± 24.8 Hz μg −1 at 69.5 ppm, a limit of detection (LoD) of 480 ppb, and excellent long-term stability, retaining 97% of the initial response after 6 months.

Session: Structural Materials

Cu Precipitation and Grain Boundary Phosphorus Segregation upon Direct Ageing of Laser Powder Bed Fusion 17-4 PH Stainless Steel

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17-4 PH stainless steel combines high strength and corrosion resistance through the precipitation of nanoscale Cu-rich precipitates (CRPs), and its excellent processability by laser powder bed fusion (LPBF) makes it a leading candidate for additively manufactured structural components. The rapid thermal cycling intrinsic to LPBF leaves a far-from-equilibrium as-built microstructure containing solute clusters, elevated dislocation densities, and metastable phases. Direct ageing takes advantage of this state by omitting the conventional solution annealing step, enabling single-step precipitation hardening at reduced cost, however, its consequences for grain boundary chemistry remain poorly understood.

In the current study, atom probe tomography and electron backscatter diffraction are combined to track nanoscale precipitation and atomic-scale segregation across eight conditions, covering two commercially distinct processing environments (~0.08 vs. ~0.35 at.% N), two laser power levels (~130 and ~170 W), and the as-built and direct aged (480 °C, 1 h) states. In the as-built state, CRPs are confined to GBs in all conditions, while the matrix retains a dense population of sub-critical Cu clusters. The N-rich environment additionally stabilises 2–5% retained austenite and develops extensive NbN precipitation along grain boundaries, where CRPs are noticeably smaller than in the low-N counterpart. Upon direct ageing, profuse intragranular CRP formation occurs in all builds, with volume fractions converging to approximately 5.5% and hardness reaching up to 469 ± 6 HV, on par with conventionally solution-annealed and peak-aged counterparts. Average CRP sizes of ~7 and ~5 nm are measured in the N-rich and low-N conditions, respectively, which may reflect faster coarsening kinetics linked to the higher dislocation density of the former.

Notably, direct ageing also induces P segregation (~0.2 at.%) at GBs exclusively in the N-rich material, placing these boundaries within the classical temper embrittlement regime. This observation is corroborated by localised P enrichment at a BCC/FCC interface near a lack-of-fusion pore in the as-built state, where extended local thermal exposure permits P diffusion. Since P-induced embrittlement is amplified at high matrix hardness, the strongest condition is potentially the most susceptible to grain boundary failure. These findings evidence that atomic-scale grain boundary chemistry must be considered when qualifying direct-aged LPBF 17-4 PH components, supporting the reliable industrial adoption of streamlined post-processing routes in additive manufacturing.

Design of Structural Colloids as Catalytic Supports

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Heterogeneous catalysts such as metal nanoparticles, are commonly immobilized on supports to prevent nanoparticle aggregation. Colloidal particles, particularly mesoporous silica particles, are one of the ideal supports due to their high specific surface area. The structures of the mesoporous silica particles need to be optimized to achieve high performance from supported catalytic nanoparticles because that performance is determined by the balance of reaction-diffusion kinetics. However, design rules for their structures have not been established.

Our research group developed structural colloids, specifically hollow silica particles that encapsulate colloidal particles within their cavities [1–3]. We demonstrated that molecules diffused through the hollow shells when the pores are larger than the molecules [4]. In the present work, to establish design guidelines for hollow mesoporous silica particles as catalytic supports, we investigated the effect of their structural parameters including shell thickness, cavity (void) diameter, and catalyst loading on the catalytic performance of encapsulated catalysts [5].

Hollow mesoporous silica particles with gold nanoparticles on the inner surface of the shells were synthesized. We precisely controlled their structural parameters: shell thickness (42–639 nm), void diameter (272–940 nm), and varied gold catalyst loading. The apparent catalytic reaction rates of each nanoreactor were evaluated using the reduction of 4-nitrophenol as a model reaction. Notably, a high apparent reaction rate was obtained for the hollow particles with a shell thickness of 85 nm and a void diameter of 895 nm, despite its low catalyst loading per hollow particle. This was because the mass transfer through the mesoporous shell and reaction rates of nanoparticles within the hollow catalytic supports were well balanced. These findings emphasize that the structural parameters of hollow catalytic supports need to be appropriately optimized for efficient utilization of encapsulated catalytic nanoparticles, considering both mass transfer and reaction kinetics.

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Super-Resolved Real-Space Evaluation of Exciton Migration in Organic Solid Materials

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Photoexcitation is a fundamental process in photochemical reactions, typically occurring through one-photon absorption resonant with molecular absorption bands. Excitation can also be induced by photons with energies lower than the absorption band through processes such as multiphoton absorption and thermally assisted photoabsorption[1]. Here, these processes are collectively referred to as upconverting photoexcitation. Such excitation schemes enable selective photoactivation using low-energy photons and can provide spatially confined excitation beyond the diffraction limit. In this presentation, we demonstrate an application of upconverting photoexcitation using upconverting nanoparticles (UCNPs) as nanoscale light sources for real-space evaluation of exciton migration in organic materials[2]. Exciton migration in conjugated molecular aggregates is a fundamental process governing the performance of photoconversion systems such as solar cells and organic light-emitting diodes. Because conjugated solids generally possess microscopic heterogeneity originating from molecular packing and aggregation structures, exciton migration strongly depends on the local environment. Direct real-space observation of where excitons are generated and how far they migrate is therefore important for understanding exciton transport beyond ensemble-averaged information obtained by conventional spectroscopy. However, diffraction-limited optical excitation makes such measurements challenging. In the present study, we employed Tm-ion-doped UCNPs (TmUCNPs) as local excitation sources. The TmUCNPs were dispersed in thin films of conjugated polymer, MEH-PPV, and individually excited with a 976-nm CW laser. The photo-excited TmUCNPs transferred the excitation energy to surrounding MEH-PPV chromophores through Förster-type resonance energy transfer, followed by exciton migration leading to fluorescence emission from lowenergy sites. Luminescence images of individual TmUCNPs and MEH-PPV were spectrally separated and analyzed by two-dimensional Gaussian fitting to determine their emission positions with nanometer precision. Although the MEH-PPV emission was spatially correlated with the TmUCNP emission, the spatial distributions of MEH-PPV emission positions around individual TmUCNPs were broader than the corresponding distributions of TmUCNP emission positions. These observations indicate that excitons generated near the UCNPs migrate through the MEHPPV film before emission from lower-energy sites. Using this approach, position-depending exciton migration lengths of up to approximately 55 nm were experimentally evaluated. Thus, UCNP-based nanoscale excitation enables real-space evaluation of exciton migration beyond the diffractionlimited excitation scheme. This approach has the potential to reveal spatial heterogeneity in exciton migration and local energy-trapping structures that are averaged out in conventional spectroscopic measurements. The upconverting nano-excitation method should be applicable to a broad range of excitonic systems and provide a useful experimental platform for investigating photonic energy-conversion processes at the nanometer scale.

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Magnetocaloric Materials for Clean and Efficient Cooling: The Promise of HoAl2 and HoB2

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Beyond Surface Modification: Designing Titanium Biointerfaces for Dentistry

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Titanium and its alloys are widely used as metallic biomaterials in dentistry because of their favorable mechanical properties, corrosion resistance, and biocompatibility. Nevertheless, their interactions with the biological environment are strongly influenced by the outermost surface rather than by the bulk material itself. Surface modification therefore provides an important route to tailor the material–biological interface. Beyond simply altering surface properties, a key challenge is to understand how engineered surface characteristics can be translated into desirable biological functions.

This presentation provides an overview of our recent efforts to design titanium biointerfaces through physical, chemical, and compositional surface engineering. Particular attention is given to the interplay among surface topography, surface chemistry, crystalline characteristics, and functional elements, and how these factors influence subsequent biological interactions. Representative approaches include laser-based surface structuring, incorporation of antibacterial metallic components, and modification of titanium oxide surfaces through nitrogen-related treatments. These studies demonstrate that changes in surface architecture and physicochemical characteristics can substantially influence biological interactions and functional responses at the material interface, while also highlighting the complexity of correlating biological outcomes with individual surface parameters.

Rather than considering surface modification as an endpoint, these findings support a biointerface-oriented approach in which processing, surface characteristics, and biological responses are systematically connected. Such an approach may provide a useful framework for the rational design of titanium-based biomaterials with tailored interfacial functions. Finally, current challenges and future perspectives for developing more predictable and functional titanium biointerfaces for dentistry will be discussed.

Data Assimilation-assisted Multi-Phase-Field Simulation of Grain Growth: Estimation of Anisotropic Grain Boundary Mobility and Energy

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Grain boundary mobility (GB) governs the kinetics of microstructural evolution during grain growth and consequently influences the properties of polycrystalline materials. Accurate computational representation and estimation of GB mobility are therefore essential for predicting microstructural evolution and establishing reliable microstructure–property relationships. In this work, a Bayesian data assimilation framework for multi-phase-field (MPF) simulation of grain growth in copper is developed accounting for uncertainty in experimental data and MPF model. In order to demonstrate the data assimilation-integrated MPF simulation, a numerical twin experiment is performed to investigate whether the time-variation of mean grain size can constrain the uncertain parameter. In the numerical experiment, an eight-grain microstructure is considered, with an effective grain-boundary mobility treated as an uncertain material parameter. Synthetic observation data of mean grain size are assimilated to the MPF simulation using an Ensemble Kalman Filter (EnKF), enabling sequential updating of the probability function of mobility and calibration of the MPF model. The estimated mobility provides a better prediction of grain growth than that using the initially estimated GB mobility, while the independently predicted microstructures closely agree with the reference microstructure. Repeated data assimilation calculation further demonstrates the consistency and repeatability of the estimation of mobility. These results demonstrate the potential of combining MPF modelling with EnKF-based data assimilation to utilize limited microstructural observation data for improved prediction of grain growth behavior. As the key extension of this work, anisotropy of GB energy and mobility will be incorporated into the MPF model. The anisotropy is described by using misorientation-dependent GB properties. This extension will provide a more physically representative computational description of grain growth and enable investigation of the interaction between anisotropic grain growth behavior and data-driven parameter estimation.

Microstructural Evolution and Mechanical Performance of High-Entropy Dual-Phase Boride-Carbide Ultra-High Temperature Ceramics

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Ultra high temperature ceramic (UHTC), particularly Zr-, Ti-, Ta-, and Hf-based high-entropy borides and carbides, are promising candidates for extreme-environment applications owing to their high melting temperatures (>3000°C), oxidation resistance, and mechanical properties (i.e., hardness > 25 GPa, Flexural strength > 560 MPa). In the present study, a (Zr,Ti,Ta,Hf)-based high-entropy boride–carbide (HEB-HEC) dual-phase ceramic and a SiC-reinforced HEB-HEC composite were developed to investigate the effect of multiphase constitution and microstructural refinement on mechanical performance. Single-phase HEB, HEC, dual-phase HEB-HEC, and HEB-HEC-SiC compositions were consolidated by spark plasma sintering at 2000 °C, achieving near-theoretical densification. Phase analysis confirmed the formation of solid-solution phases in the HEB and HEC, while the dual-phase compositions exhibited a homogeneous distribution of boride and carbide phases. The incorporation of secondary phases effectively suppressed grain coarsening via Zener pinning, resulting in significant microstructural refinement. The refined multiphase architecture, together with the increased density of grain and phase boundaries, resulted in a favorable combination of strength, hardness, and fracture resistance. The HEB-HEC ceramic exhibited a flexural strength of ~595 MPa and fracture toughness of ~4.1 MPa·$m^{1/2}$, whereas SiC incorporation enhanced the fracture toughness to ~4.9 MPa·$m^{1/2}$ and microhardness to ~27.3 GPa, with a flexural strength of ~580 MPa. The improved fracture resistance is attributed to grain refinement and the increased population of boride–carbide and carbide-SiC interfaces, which promote crack deflection and impede crack propagation. These findings demonstrate that multiphase and interface engineering can effectively tailor the mechanical response of high-entropy UHTCs for demanding aerospace and hypersonic applications.

Keywords: High-Entropy UHTCs; Dual-Phase Ceramics; Boride–Carbide; Microstructural Refinement; Zener Pinning; Crack Deflection; Fracture Toughness

Electric-Field Directed Assembly in Fluorine-containing Block Copolymer Films

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The pursuit of sub-10 nm feature sizes in block copolymer (BCP) lithography requires a large Flory–Huggins interaction parameter (high χ) combined with a low degree of polymerization (low N); however, such strongly immiscible systems commonly suffer from preferential surface wetting that enforces parallel orientation and necessitates top-coats or neutral underlayers. Overcoming this orientation problem without introducing additional processing layers remains a central challenge in the field. In this study, a silicon- and fluorine-containing BCP, polydimethylsiloxane-b-poly(2,2,3,3,3-pentafluoropropyl acrylate) (PDMS-b-PPeFPA), was designed so that the two blocks possess nearly identical surface energies (γPDMS ≈ γPPeFPA) while retaining a high χ arising from the strong chemical dissimilarity between the siloxane and fluoroacrylate segments. This deliberate balancing of interfacial

energies established dual-neutral interfaces at both the substrate and the free surface, enabling perpendicular lamellar orientation with sub-10 nm half-pitch dimensions without any additional top-coat or neutral layer. The low glass transition temperatures (Tg) of both blocks further promoted chain mobility and defect relaxation during selfassembly, allowing well-ordered microdomains to form under mild thermal annealing. The orientation behavior was systematically examined across substrates of differing surface chemistry, including native SiOx, hydrogen-terminated Si, and copolymer-coated surfaces. Robust perpendicular alignment was consistently obtained on random-copolymer-modified substrates, where the minimized interfacial selectivity suppressed preferential wetting and reinforced the neutral boundary condition. Beyond spontaneous perpendicular ordering, the pronounced dielectric contrast between the silicon-rich PDMS and the fluorine-rich PPeFPA domains was exploited to realize two-dimensional directed assembly: application of a lateral electric field aligned the lamellae unidirectionally, transforming fingerprint-like textures into laterally ordered arrays and demonstrating electroresponsive control over in-plane orientation. Subsequent O_2 plasma etching selectively oxidized the PDMS block into a robust silica-like framework while removing the organic PPeFPA, yielding high-resolution, unidirectional air–inorganic nanoarrays directly applicable to nanofabrication. To overcome the limited mechanical and thermal stability arising from the low Tg of both constituent blocks, a second-generation system was developed in which the fluorinated acrylate block was replaced by a methacrylate analogue, poly(2,2,2-trifluoroethyl methacrylate) (PTFEMA). The resulting PDMS-b-PTFEMA copolymers were designed to preserve the high χ and interfacial neutrality of the parent system while introducing greater chain rigidity through the methacrylate backbone, thereby improving domain stability and process durability. These modified copolymers, currently under investigation, extend the design concept toward more manufacturable platforms. Collectively, this work establishes a molecular design strategy that simultaneously integrates interfacial energy balance, dielectric contrast, and chain rigidity within a single highly immiscible BCP framework. By decoupling the requirement for high χ from the persistent problem of surface-energy-driven parallel orientation, the approach realizes perpendicularly oriented, electrically directable, sub-10 nm lamellar nanostructures and offers a versatile route toward next-generation nanolithographic and nanofabrication technologies.

Fast Fabrication of Eu 2 O 3 -Doped Silicate Glass Scintillator Prepared by Microwave Melting Technique

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A series of Eu_2O_3-doped SiO_2:Na_2O:BaO:ZnO glasses was fast prepared using a microwave melting technique to investigate their structural, photoluminescence (PL), and radioluminescence (RL) properties for scintillation application. The amorphous nature of the samples was confirmed by X-ray diffraction (XRD). UV–Vis–NIR spectra provided information on optical transparency and Eu^{3+}-related absorption features. Under optical excitation (λ_{ex} = 394 nm), the glasses exhibited characteristic Eu^{3+} emission, and the PL intensity increase with increasing Eu_2O_3 concentration, indicating enhanced activation of luminescent centers. The emission chromaticity lay in the red region with CIE (x, y) = (0.6458, 0.3538). Changes in the local symmetry around Eu^{3+} ions were evaluated using the electric-dipole to magnetic-dipole (ED/MD) intensity ratio and further supported by Judd-Ofelt (JO) analysis. Under X-ray excitation, the samples showed scintillation light, with maximum intensity at 3.00 mol% and integral radioluminescence efficiency is 8.9% relative to a commercial BGO scintillator. These results demonstrating promising potential for scintillation and x-ray screen.