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Meeting Abstracts

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Keynote Session

Improving Mechanical Properties of Carbon Fiber Reinforced Epoxy Laminate, Its Self-healing and Recycling

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Abstract

In this work, mechanical properties of a carbon fiber (CF) reinforced epoxy (Ep) (CFRE) laminate are significantly improved, and self-healing properties are imparted to it. This laminate is also successfully recycled using our proprietary environment friendly solution SalSO™. A polyetherimide termed as BA is prepared by mixing 4,4'-(4,4'-Isopropylidenediphenoxy) bis(phthalic anhydride) and 4-aminophenyl disulfide. A functionalized graphene oxide termed as hGO is also prepared. hGO is tagged to BA, termed as BAhGO. CF reinforcement is sized with a small amount of BAhGO, and a small amount of hGO is dispersed in Ep matrix. The resultant laminate termed as BAhGO-CFRE-hGO exhibits 44% increase in flexural strength (FS) and 41% increase in interlaminar shear strength (ILSS) over neat CFRE laminate. It also exhibits 61% self-healing efficiency in ILSS. BAhGO-CFRE-hGO laminate is dissolved in SalSO™ with almost 100% recovery of matrix Ep, termed as rEp, and reinforcement CF, termed as rCF. rEp is used as hardener for Ep, and the resultant Ep, termed as Ep-rEp, exhibits 3% higher tensile strength than Ep prepared using conventional hardener. The laminate fabricated by using Ep-rEp matrix, termed as Ep-rEp-CFRE, exhibits 17% higher FS and 13% higher ILSS than CFRE prepared using Ep matrix.

Microstructure Characterization for Failure Analysis of Polymer Matrix Composites with Manufacturing Defects

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Abstract

Polymer matrix composites are manufactured by a variety of methods, ranging from labor-intensive hand layups to fully automated techniques employing robotics. Depending on the degree of control in the manufacturing process different defects appear in the final product. These defects can be described as deviations from the intended morphology of the internal structure of a composite. Examples are non-uniform fiber distribution and fiber misalignment, imperfect fiber-matrix bonding, and matrix voids. All such defects can be initiators of local damage that can lead to deterioration of the composite performance. This presentation will discuss a strategy for performance evaluation of composite structures accounting for the severity of manufacturing defects. A statistical methodology for construction of representative volume elements combined with local stress and failure analysis applicable to polymers will be presented. Certain fundamental issues concerning descriptors of randomness and non-uniformity will also be addressed.

Treating Cancer Through a One Medicine Vision

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Abstract

The successful translation of emerging cancer therapeutics and their combination with therapeutic devices remains limited by the inability of conventional preclinical models to fully capture the biological complexity of human disease. The One Medicine paradigm addresses this challenge by integrating naturally occurring cancers in companion animals into the translational pipeline, creating a continuum between laboratory discovery and human clinical investigation. At the University of Texas Southwestern, we have established a multidisciplinary One Medicine program that integrates engineering, comparative oncology, immunology, and clinical oncology to investigate high-intensity focused ultrasound (HIFU) as a platform for improving cancer therapy. Rather than serving solely as a local ablative modality, HIFU is being explored as a versatile tool capable of enhancing intratumoral drug delivery, improving the performance of nanoparticle- and liposome-based therapeutics, promoting antigen release, and augmenting anti-tumor immune responses. By leveraging distinct HIFU modalities, including mild hyperthermia, thermal ablation, and histotripsy, we seek to define how acoustic energy can be tailored to maximize therapeutic efficacy while minimizing normal tissue injury. This talk will provide insights into how the One Medicine approach is accelerating the development of HIFU-enabled combination therapies and advancing more effective chemo-immunotherapy strategies for both veterinary and human cancer patients.

Intrinsic Topological Weyl Phase Transition Induced by a Magnetostructural Transformation in a Kagome Magnet

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Abstract

Topological phase transitions provide a unique window into the interplay between structure, magnetism, and Weyl physics in magnetic Weyl semimetals. However, realizing an intrinsic Weyl phase transition between two distinct Weyl states near room temperature remains challenging. Here, we demonstrate that a magnetostructural transition effectively induces such a transition in the kagome magnet Mn_3Ga. High-resolution neutron diffraction, magnetization characterizations and first-principles calculations reveal that Mn_3Ga undergoes a chiral antiferromagnetic transition below 485 K, followed by a magnetostructural transition to a monoclinic structure with highly canted antiferromagnetic order near room temperature. These cooperative changes in lattice and magnetic symmetries reorganize Weyl nodes, driving a transition from a primary type-II Weyl state to a distinct Weyl state, accompanied by dramatic variations in the anomalous Hall effect and appearance of topological Hall effect. Our findings open a new pathway for discovering novel topological Weyl states and potential spintronic applications.

Mechanistic Underpinnings of Polysulfide Formation and Evolution of Interfacial Solid Electrolyte Interphase Layer During Lithium-sulfur Interaction: Effect of Catalysts and Electrolyte Additives

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Abstract

The lithium-sulfur battery concept is promising for the subsequent generation of energy storage due to its distinct advantage of high theoretical capacity (1675 mA/g) and energy density (2600 Wh/gm). Yet the formation of polysulfides as intermediate discharge products (Li_2S_n, $4 < n < 8$) and their dissolution result in the loss of active material and ultimate deposition at the anode. This shuttle phenomenon gives rise to irreversible loss of active material, rapid capacity fading, low coulombic efficiency and short cycle life with an ambiguity of its mechanism. To our knowledge, we are the first to employ *in situ* characterization techniques, including Raman spectroscopy and X-ray absorption spectroscopy (XAS), to investigate the evolution of kinetics with various electrolyte systems. This work presented the formation change of polysulfide intermediates at various fluorinated additives environments with different formulas and compositions based on *in-situ*/operando Raman spectroscopy. The Raman results revealed that the long-chain polysulfide conversion (400 cm^{-1}) was pushed forward, and an increase in the concentration of short-chain polysulfide (453 cm^{-1}) appeared when fluorinated carboxylate ester-based electrolyte was used at its optimized formula compared to the baseline. Cyclic voltammetry results correspond to the chemistry evolution proposed by Raman. *In-situ* XAS was also conducted on the sulfur K-edge to monitor the polysulfide intermediates' formation. X-ray fluorescence mapping on the cathode and anode also confirmed that the sulfur shuttle phenomenon was significantly suppressed in fluorinated carboxylate ester-based electrolytes by changing the sluggish kinetics. This presentation will also show results of catalytic effect of single atom catalysts in the form of transition metal coordinated with nitrogen embedded in a carbon matrix hereby referred to as M-N-C catalyst. Sulfur interactions with metal center will be presented both from the point of view of *in situ*/operando Raman and X-ray absorption data using tender X-ray facility at the National Synchrotron Light Source-II at Brookhaven National Laboratory (Upton, NY).

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Next Generation Systems for Meeting the High Energy Density Challenge

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Abstract

Energy storage is currently the main engine vital for an energy independent global economy currently still very much dependent on exploiting into the earth's natural reserves aided by natural oil and gas exports. The lithium-ion (Li) battery chemistry has emerged at the forefront of secondary rechargeable battery systems and has witnessed burgeoning and significant research activity ever since the commercialization of the first Li battery in 1990. There

have been alarming advances in all areas of cathodes, anodes, and electrolytes. Despite much progress, lithiated transition metal oxides and carbon remain the ideal mainstream systems that have made it into the commercial systems deployed in electric vehicles (EVs) at present. The search for higher energy density systems has drawn the attention of Li-air and Li-sulfur (S) systems recently. The Li-S systems are of particular interest due to the potential of achieving 500 $Whkg^{-1}$, a "holygrail" in energy density for next generation EVs matching and exceeding the performance metrics of the internal combustion engine. This presentation will discuss all the materials challenges in generating high-energy density cathodes and anodes as well as electrolyte additives to meet the grand challenge of 500 $Whkg^{-1}$. Efforts made in the areas of new S confinement materials with ability to confine high S loadings combined with unique electrocatalysts exhibiting the propensity to trap polysulfides while also catalyzing the formation of Li_2S will be discussed. Concurrently, research directions in generating new dendrite-free anodes, and current collectors as well as electrolyte additives matching the cathode performance will be outlined.

Integrated Photovoltaic and Photothermal Strategies for Continuous Energy Harvesting from Sunlight and Indoor Light Emitting Diode Lighting in Buildings

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Abstract

This study integrates photovoltaic (PV) and photothermal strategies to enable continuous energy harvesting from sunlight and indoor lighting, addressing limitations of conventional solar systems in urban environments. Semi-transparent cadmium telluride PV cells with average visible transmittance of 40 - 80% demonstrated power conversion efficiencies (PCEs) under light emitting diode (LED) illumination comparable to sunlight, with a stacked five-panel configuration reaching 20.51% PCE. Silicon-based PV (Si PV) panels under low-intensity indoor LED lighting (~1.4 mW/cm^2) achieved PCEs up to 31% and photon recycling efficiencies of 37.23%, producing cumulative energy outputs of 0.19 kWh (series) and 0.32 kWh (parallel) over 20 h. Indoor LEDs provide a continuous, diffuse, underutilized energy source, captured by semi-transparent PV panels integrated into building facades and windows, supporting energy-neutral buildings and powering cooling and electronic systems during nighttime or low-light conditions. Complementing electricity generation, a transparent photothermal radiator of plasmonic Fe_3O_4@$Cu_{2-x}S$ thin films efficiently converts ultraviolet and infrared components of sunlight and indoor lighting into heat. Experiments in a diffused light photothermal box demonstrated temperature increases above 50 °C under simulated indoor conditions. These combined technologies create a multifunctional platform harvesting both electrical and thermal energy from natural and artificial light, enabling sustainable, self-powered building systems and efficient use of otherwise wasted photons in urban environments.

Session I: Advanced Functional, Structural and Sustainable Materials

Thermoplastics Composites Made by Non-pressure Technologies

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Abstract

Adhesion between matrix and a filler is the key parameter to obtain proper mechanical properties of composites. Special sizings have been developed and frequently used thermoset matrix (epoxy, polystyrene, etc.) which enable production of composites with superior properties. Such composites are nowadays applied in various branches of industry including automotive and/or aircraft production. Improvement of interfacial adhesion in thermoplastic matrix based composites is still an open question. Grafting of polyolefin matrix with maleic anhydride is usually used to enhance the interfacial adhesion in thermoplastic composite. Plasma treatment is an ecological alternative. The industrial-scale device for plasma treatment of a powder material has been developed by the company SurfaceTreat Inc. Experimental results of thermoplastic composites made from thermoplastic polyethylene matrix and several types of reinforcement with natural fibers, glass fibres and/or carbon fibers will be presented. An application of the glass-fibre reinforced composite for industrial rotomolding production of insulating containers and a sports kayak will be demonstrated.

Integrated Shielding: Combining Structure, Processability and Radiation Protection in a Single Fibre

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Abstract

Lightweight radiation shielding remains a key challenge in spacecraft design, where conventional metallic enclosures and particle-filled systems impose penalties in mass, manufacturability and geometric flexibility. This work presents a fibre-integrated shielding concept based on continuous glass fibres coated with metals like bismuth, enabling radiation attenuation to be incorporated directly into textile and composite feedstocks rather than added as a secondary layer. Because bismuth is intrinsically brittle and not processable via conventional fibre routes, the approach relies on an inline coating technology that applies bismuth directly to continuous filaments while preserving textile processability. The resulting fibres can be integrated into composite architectures combining shielding capability, structural function and compatibility with established manufacturing processes. Shielding performance is evaluated using GEANT4 simulations based on representative low earth-orbit radiation spectra. Preliminary results indicate that the proposed composites can achieve approximately 25% performance increase or mass reduction respectively at comparable total ionising dose performance relative to aluminium in the studied configuration. This fibre-level integration enables drapable, tailorable shielding structures suitable for complex geometries and multifunctional applications. The work demonstrates a scalable pathway towards composite materials in which radiation protection, structural performance and manufacturing compatibility are co-designed at the filament level, providing a promising route for next-generation spacecraft structures and electronic protection concepts.

Degradation Physics and Molecular Modeling for Nanomaterials

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Abstract

All fabricated materials are metastable and will degrade with time. This is a consequence of the material changing in an effort to reach a lower Gibbs potential. Thus, for a material to be successful/reliable, the degradation rate must be fully comprehended. Toward this end, it is very important to understand when macroscopic models can no longer be used, and a more microscopic approach (molecular approach) must be used for nanomaterials. During this presentation, we will use the example of dielectric thickness scaling in metal-oxide-semiconductor field-effect transistor. In the semiconductor industry, gate dielectric thicknesses have decreased from ~ 50nm (1980s) to only a few nanometers today. In the process of scaling the silicon dioxide gate dielectric thickness, microscopic (molecular) models were required to fully understand the changes in degradation physics. These models revealed that the dielectric breakdown strength improves with thickness reduction; high-k dielectrics exhibit lower breakdown strength; only dielectrics with polar molecular bonding experience time-dependent dielectric breakdown (TDDB); and the TDDB lifetime increases with frequency. It will be shown that molecular models must be used to fully explain the degradation physics for nanomaterials.

Valorization of Polyurethane Waste via Pyrolysis-derived Carbon Black in Elastomeric Polyurethane Systems

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Abstract

Polyurethane (PU) waste represents a significant environmental challenge due to its high production volume and limited recycling options. This study investigates a material-oriented circular recycling strategy in which PU waste is converted into a functional pigment via thermochemical pyrolysis and reutilized in elastomeric PU systems. The aim is to evaluate the compatibility of pyrolysis-derived recycled carbon black with conventional elastomeric PU formulations used in automotive applications. PU waste was subjected to controlled pyrolysis to obtain a carbon-rich powder, which was processed into a black pigment. The pigment was incorporated at 4 wt% into an elastomeric PU formulation designed for automotive floor mat applications. For an accurate comparative assessment, both the standard and recycled pigment-modified elastomeric PUs were synthesized using identical base chemistries, comprising polypropylene glycol, polyether polyol, and 4,4′-methylenediphenyl diisocyanate. The initial isocyanate index was set at 15% and subsequently optimized to 16% to achieve the targeted elastomeric stiffness and curing behavior. Colorimetric properties were evaluated using spectrophotometric measurements based on L^*, a^*, and b^* coordinates. The recycled pigment-containing elastomeric PU exhibited color values closely matching those of the reference formulation. Mechanical durability was assessed via Taber abrasion testing in accordance with ASTM D4060 (H-18 wheel, 1000 g load, 60 rpm, 1500 cycles). Both formulations demonstrated comparable abrasion resistance, with mass loss values of approximately 0.4%. The results confirm that pyrolysis-derived recycled carbon black is chemically and mechanically compatible with elastomeric PU systems and can effectively replace conventional pigments. This approach provides a viable pathway for sustainable PU waste valorization within high-performance elastomeric applications.

Session II: Nano, Electronic and Functional Materials

Crystal Field Theory as a Sufficient Framework for Magnetocrystalline Anisotropy Prediction in Spinel Ferrites

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Abstract

Quantitative design of spinel ferrites for targeted magnetocrystalline anisotropy (K_1) requires a framework that is physically justified and practically tractable. This presentation establishes that crystal field theory (CFT), operating through the one sub-lattice positive-K_1 energy formalism, is necessary and sufficient for that purpose. Ligand field theory (LFT) and density functional theory occupy no intermediate role within the validated composition space. The justification rests on the energy hierarchy Δ_{CF} (1 - 2 eV) $\gg \lambda_{SO}$ (0.05 – 0.10 eV) for substitution of first-row transition-metal ions on regular spinel sites. This separation renders CFT the dominant perturbation, allows spin-orbit coupling as a secondary correction, and validates K_1 as a linear superposition of single-ion contributions. The central design contrast is between iron (Fe^{3+}) (d^5, $^6A_1$, L = 0, negligible anisotropy) and cobalt (Co^{2+}) (d^7, $^4T_1$, unquenched orbital moment, $k_{Co} \approx +2.5 \times 10^5$ J/m^3). Validation against five nickel-zinc-cobalt compositions yields agreement within ~±10% using a single nephelauxetic scaling parameter. LFT adds no predictive improvement: covalency shifts Δ_{CF} isotropically, charge-transfer states lie 3 - 5 eV above the ground state, and isotropic corrections cancel by symmetry in the K_1 energy difference; the leading anisotropic LFT term enters only at third order in $\lambda_{SO}/\Delta_{CF} \approx 0.05$. Validity boundaries are quantified: CFT linearity holds within ~ ±10% for Co^{2+} loadings below ~ 8 mol% and the Stevens operator formalism is required only when rare-earth dopants invert the energy hierarchy. These results provide the theoretical foundation for the Harris six-step predictive design algorithm for K_1-targeted ferrite development.

Twisted van der Waals Integration of Thin Magnetic Layers with Magnetic Skyrmion and Magnetic Tunneling Junctions for Next-generation Memory

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Abstract

Twistronics, a novel engineering approach involving the alignment of van der Waals (vdW) integrated two-dimensional materials at specific angles, has recently attracted significant attention [1]. Novel non-trivial phenomena have been demonstrated in twisted vdW junctions (i.e., magic angle), such as unconventional superconductivity, topological phases and magnetism. However, there have been only few reports on integrated vdW layers with large twist angles θ_t, such as twisted interfacial Josephson junctions using high-temperature superconductors [2]. Herein, we assemble vdW homo-junctions of the novel thin-magnetic flakes, Fe_3GeTe_2 (FGT) [3], with large θ_t ranging from 0° to 90°, without inserting any tunnel barriers (Figure 1) [4]. Nevertheless, we discover that these vdW homojunctions

exhibit tunnel-magnetoresistance (TMR) like behavior (pseudo-TMR (PTMR) effect) with the ratios highly sensitive to the θ_t values (Figure 2). We reveal that the vdW gap at the junction interface between the twisted FGT layers can behave like a tunnel barrier and the θ_t serves a control parameter for PTMR by drastically varying magnitudes of the lattice-mismatch and the subsequent appearance of antiferromagnetic (AFM) spin alignment. First-principles calculations considering vacuum gaps indicate strong dependence of TMR on the θ_t driven by the 6-fold screw rotational symmetry of bulk FGT. While the PTMR ratios are still small, our previous theory predicts that the largely dissimilar AFM spin alignment and magnetic skyrmions unique to the FGT (or FGaT) layers can lead to giant TMR effects (>> 1000 %) for the non-twisted FGT/vacuum gap/FGT TMR structure even at room temperature [5]. Further results, including these skyrmion-based TMRs on tungsten ditelluride/FGT or FGaT figure 3, are presented at the conference.

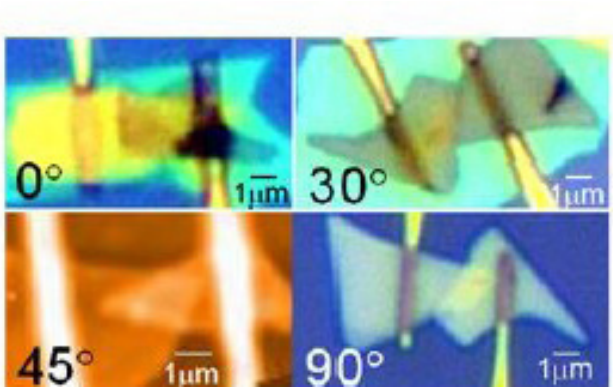


Figure 1: Twist-angle (θt) dependent images of vdW-integrated two FGT flakes.

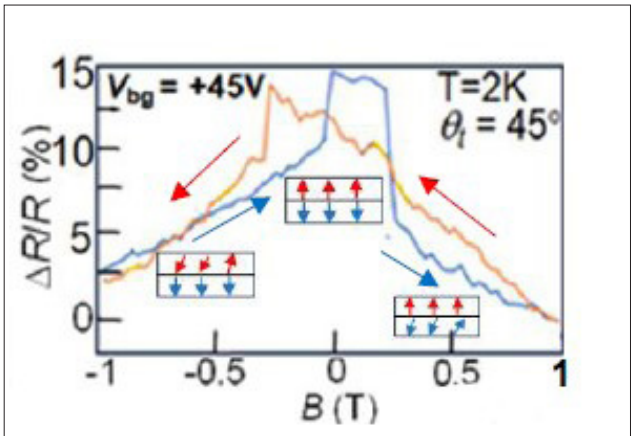


Figure 2: PTMR peak (blue curve) observed at θt of 45° in figure 1 under back gate voltages (Vbg) of +45 V. Schematic insets mean the lattice-mismatch derived antiferromagnetic (AFM) spin alignment of the two flakes.

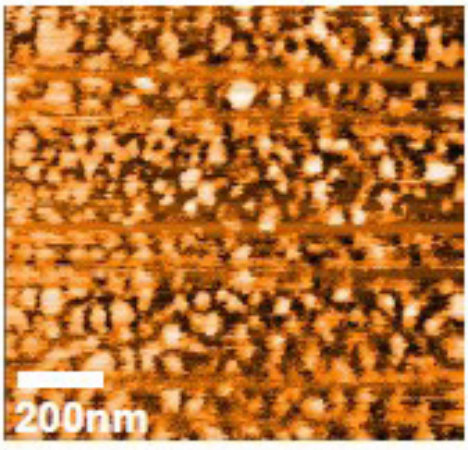


Figure 3: Magnetic force microscopy image of room-temperature magnetic skyrmions in a FGaT flake.

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Chemical Stabilization of Niobium Interfaces for High-coherence Superconducting Transmon Qubits

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Abstract

Dielectric loss arising from two-level systems at surfaces and interfaces remains a major limitation to coherence in superconducting transmon qubits. Niobium (Nb), a widely used material in superconducting quantum circuits, readily forms native oxides under ambient conditions, leading to lossy dielectric interfaces that degrade device performance. Here, we demonstrate a robust and scalable fabrication strategy for chemically stabilizing Nb surfaces and mitigating further oxidation, including protection of both surface and sidewall regions relevant to superconducting transmon qubits. High-purity Nb films were fabricated with bulk-like superconducting transition temperatures (T_c = 9.30 ± 0.10 K). We show that a thin platinum (Pt) encapsulation layer, deposited after native oxide formation, can be transformed by thermal annealing into a Nb-Pt alloy at the surface. Spectroscopic and microscopic analyses confirm the formation of a chemically stable metallic alloy layer and its ability to suppress further oxide growth. Ab initio simulations reveal the atomic-scale rearrangement and electronic-structure evolution associated with Pt incorporation into native Nb oxide, providing insight into the stabilization mechanism. This approach offers a materials pathway for engineering chemically robust Nb interfaces, including sidewalls, toward higher-coherence superconducting transmon qubit architectures.

Enhancing Sustainable Photocatalytic Carbon Dioxide Conversion to Methane via Molecularly Doped Graphitic Carbon Nitride Nanostructured Materials

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Abstract

The development of efficient photocatalysts for solar energy driven carbon dioxide (CO_2) conversion has attracted significant attention as a sustainable strategy to address global energy and environmental challenges. Developing graphitic carbon nitride (g-C_3N_4) based materials have emerged as promising photocatalysts due to their suitable band position, chemical stability and visible light responsiveness. In this research work, our research group developed engineered sulfur and 2,4-diaminopyrimidine (DAP) doped C_3N_4 materials for efficient CO_2 reduction under visible light irradiation. The synthesized materials were systematically characterized using advanced analytical techniques including X-ray diffraction, X-ray photoelectron spectroscopy, scanning electron microscopy, transmission electron microscopy, energy-dispersive X-ray spectroscopy, photoluminescence spectroscopy, and electrochemical studies to investigate their structural, morphological, and electronic properties. The photocatalytic CO_2 reduction performance of boron carbon nitride (BCN), sulfur doped carbon nitride (SCN) and DAP modified SCN photocatalysts was systematically investigated and evaluated based on CO_2 conversion rates (μmol g^{-1}). Pristine BCN exhibited a

relatively low CO_2 reduction activity of 0.02702 μmol g^{-1} due to its limited visible-light absorption and rapid recombination of photogenerated charge carriers. Sulfur incorporation significantly enhanced the photocatalytic performance, with SCN achieving a CO_2 conversion rate of 0.09299 μmol g^{-1}, indicating improved charge transport and broadened visible-light harvesting capability. Among all synthesized materials, 7DSCN showed the highest CO_2 reduction activity of 0.13686 μmol g^{-1}. The superior performance of 7DSCN is attributed to the formation of an efficient donor-π-acceptor electronic structure, which promotes rapid charge transfer, suppresses electron-hole recombination, prolongs charge carrier lifetime, and enhances CO_2 adsorption and activation, leading to efficient solar-driven methane generation.

Vapor-deposited Nanocoatings for Rapid and Anti-fouling Membrane Distillation

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Abstract

Membrane distillation (MD) is a thermally driven separation technology with strong potential to utilize low-grade or waste heat, produce high-purity freshwater, and treat high-salinity feeds. However, its practical deployment is limited by low permeate flux, pore wetting, and membrane fouling, which compromise efficiency and long-term stability. This presentation introduces a vapor-deposited nanocoating platform that enhances mass transport and fouling resistance by precisely engineering membrane interfaces without compromising pore structure. Using a solvent-free technique called initiated chemical vapor deposition, ultrathin hydrophobic, hydrophilic, and omniphobic nanocoatings were conformally deposited onto porous substrates. The solvent-free coating process allows precise surface modification while preserving membrane microstructure. As a result, large-pore-size membranes (up to 2.0 μm) can be stably employed in MD, enabling stable MD operation with >99.99% salt rejection and 48 - 73% higher permeate flux compared to smaller-pore counterparts. Furthermore, integration of hydrophilic and omniphobic layers creates Janus architectures that resist emulsion wetting and organic fouling. Under highly saline and oil-containing conditions, the modified membranes maintained stable flux and excellent desalination performance, demonstrating strong resistance to oil-induced wetting and foulant adhesion. By decoupling surface chemistry from bulk morphology, vapor-deposited nanocoatings provide a scalable strategy to overcome the flux-stability trade-off in MD and advance the design of next-generation MD membranes.

Session III: Materials Design, Modeling and Characterization

Strain Localization in Austenitic Stainless Steels by Atom Force Microscope

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Abstract

Topographic analysis of shear bands (SBs) in austenitic stainless steels, deformed *in situ* under tension up to 0.03 plastic strain, reveals that SBs nucleate first in the grain bulk. A SB can accommodate 6 to 133 times the macroscopic deformation. The number of detected SBs saturates very early at 1% plastic strain, which coincides with the peak of kinematic hardening in this material. Beyond this point, plasticity is primarily accommodated through elongation of SBs. The accommodated shear and SB thickness vary between grains but remain nearly constant during the tensile test. With increasing deformation, SBs impinge on grain boundaries, leading to strong interactions that follow different scenarios identified through atom force microscope measurements. In parallel, an original theoretical framework is developed to interpret SB topography in relation to local shear and dislocation mechanisms. It is shown that the number of emerging dislocations per SB is constant, independent of grain orientation or neighbourhood. This suggests that dislocation sources within a single SB emit an approximately constant number of dislocation loops before extension. Additionally, the quasi-static elongation of SBs adheres to a kinematic condition under which the Geometrically Necessary Dislocation (GND) density at the SB ends remains constant during elongation. Detailed analysis of SB topography in intergranular regions sheds light on the mechanisms governing SB interactions with grain boundaries. Slip transmission is found to require large GND storage against grain boundaries before transmission. The other types of interactions are analyzed too, revealing some surprising features of dislocation interaction with grain boundaries.

A Two-scale Crystal Plasticity and Artificial Intelligence Surrogate Framework for Predicting Early Fatigue Damage in Additively Manufactured Materials

Jiahao Cheng*

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Abstract

Predicting fatigue crack initiation from manufacturing-induced microstructural features is a central challenge in computational materials science. This challenge is especially pronounced in additively manufactured (AM) alloys, where process-induced heterogeneity in microstructure and surface condition can strongly affect fatigue resistance. In this work, a two-scale crystal plasticity finite element (CPFE) framework coupled with a Chaboche-type fatigue damage model is developed to simulate microcrack initiation and early-stage fatigue damage under low-cycle fatigue loading in laser-powder bed fusion nickel-based alloys. To quantify the role of AM-induced features, synthetic microstructures and surface conditions spanning a broad range of process-relevant characteristics are constructed for large-scale simulations. The resulting CPFE-based fatigue life data are statistically analyzed, and an artificial intelligence-based surrogate model is developed to rapidly predict fatigue crack initiation and early propagation from key microstructural and surface descriptors. This framework combines physics-based simulations with data-driven modeling to enable rapid prediction of fatigue life while providing mechanistic insight into how AM process-induced microstructural features influence fatigue crack formation and early propagation.

Accelerated Development of Materials Using High-throughput Strategies and Artificial Intelligence/Machine Learning

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Abstract

The dramatic acceleration of the materials innovation cycles is contingent on the development and implementation of high throughput strategies in both experimentation and physics-based simulations, and their seamless integration using the emergent artificial intelligence/machine learning (AI/ML) toolsets. This talk presents recent advances made in the presenter's research group, including: (i) a novel information gain-driven Bayesian ML framework that identifies the next best step in materials innovation (i.e., the next experiment and/or physics-based simulation to be performed) that maximizes the expected information gain towards a specified target (e.g., optimized combination of material properties, refinement of a material constitutive response), (ii) computationally efficient versatile material structure analyses and statistical quantification tools, (iii) formulation of reduced-order process-structure-property models that enable comprehensive inverse solutions needed in materials design (e.g., identifying specific compositions and/or process histories that will produce a desired combination of material properties), and (iv) high throughput experimental protocols for multi-resolution (spatial resolutions in the range of 50 nm to 500 microns) mechanical characterization of heterogeneous materials in small volumes (e.g., individual constituents in composite material samples, thin coatings or layers in a multilayered sample). These recent advances will be illustrated with case studies.

Artificial Intelligence-guided Predictive Modeling of Lanthanide Separation Using Ligands in Capillary Electrophoresis

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Abstract

The separation of lanthanides is essential for critical metal supply chains. However, the separation challenge remains a bottleneck due to subtle chemical differences across the lanthanide series. These challenges motivate the development of predictive, data-driven modeling approaches. In this work, we present a layered, data-driven framework to predict and interpret lanthanide separation behavior in capillary electrophoresis by integrating empirical modeling, physics-informed features, and chemistry-aware descriptors. We first establish a baseline predictive model using ligand identity, concentration, and metal pair, achieving moderate accuracy ($R^2 \approx 0.74$). To incorporate domain knowledge, we introduce physics-informed features derived from electrophoretic mobility and peak width, leading to a substantial improvement in predictive performance ($R^2 \approx 0.94$). These results indicate that separation resolution is strongly governed by underlying transport processes. Next, we develop a machine learning model using ligand descriptors, including pKa, denticity, stability constants and chemical descriptors. This approach achieves high predictive accuracy for mid- and heavy-series lanthanides ($R^2 > 0.87$), while revealing limitations for light lanthanide pairs. Feature importance analysis further uncovers a mechanistic transition across the series, with separation behavior shifting from mobility-dominated to thermodynamically controlled regimes. This framework enables artificial intelligence-guided exploration of ligand selection and separation conditions, supporting rapid optimization of separation performance and reducing experimental burden in critical metal processing.

Contrastive Diffusion Models Enable Targeted Discovery of Lung-specific Cell-penetrating Peptides

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Abstract

Cell-penetrating peptides (CPPs) are important carriers for delivering therapeutic molecules into cells. However, identifying functional and application-specific CPPs remains challenging. In this study, we develop a deep learning framework to classify CPP and non-CPP sequences. The model combines gated recurrent units, transformer-based attention, and attention pooling. This design helps capture both local sequence patterns and long-range dependencies. Our model learns compact and informative representations of peptide sequences. These representations are then used to organize the peptide feature space. This allows us to explore new peptide candidates with desired functional properties. The approach enables guided discovery without relying only on known templates. From a material and drug delivery perspective, this framework supports the design of efficient peptide carriers. It helps in selecting CPPs for packaging and delivering therapeutic cargo such as siRNA, mRNA, and proteins. Our model reduces experimental effort and improves formulation design. Overall, this work shows how sequence-based learning can accelerate CPP discovery. It also supports better material selection for targeted drug delivery and packaging applications.

Glycographer: Atomistic Binding Landscape Characterization Towards Targeted Glycan Nanocarrier Design

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Abstract

The antibody-like targeting capabilities and unrivaled biocompatibility of glycans have made them a highly sought after material for use in drug delivery systems (DDSs) since the late 2000s. Additionally, the past two decades have proven that simulation of glycosylated systems can overcome the barriers inherent to experimental glycobiology which often cannot provide atomistic resolution models for design. While computational simulation and design of glycosylated DDSs have seen some advancements in recent years, a comprehensive methodology capable of accommodating the extensive design space and multivalent binding phenomena inherent to targeted glycomaterials has not yet been fully established. It is here that we propose a computational platform equipped to generate energy-optimized, targeted de novo glycoligands via a novel PyRosetta-based protocol towards their actualization as a smart biomaterial for use in nanomedicine. This end-to-end simulation pipeline employs dynamic grid box-sampled docking of glycan fragment probes to characterize per-fragment interaction energy landscapes across the putative binding site of a known receptor. Superimposed landscapes are then used to design candidate sequences using fragment-linking and "anchor-and-grow" approaches. All computational processes including their dependencies are open-source and constructed entirely in Python, leaving open the prospect for easily accessible deployment through package managers like Anaconda. This methodology promises to extend the application of glycan sequence optimization and atomistic modeling to biopharmaceutical materials development.

Toward Glycoprotein-inspired Biomaterials: Improved Implicit Solvent Modeling of Glycans

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Abstract

Nature offers a range of soft materials, including lubricating mucus hydrogels, polysaccharide rich algal gels, and marine adhesive protein coatings. These materials excel in barrier, lubrication, and adhesion because they are built from densely hydrated glycan-protein networks. Such glycoproteins form dynamic, water-rich assemblies with

significant biomedical potential, especially for developing new biopolymers. While such glycoprotein-rich materials are highly promising, their atomistic behavior remains difficult to characterize, despite intensive experimental and computational efforts. Explicit solvent simulations of these highly hydrated environments require immense computational resources, particularly because glycoproteins are large and heavily glycosylated. In this study, we improve implicit solvent which treats water as a continuum medium, as a pathway toward efficient, molecular-level understanding of glycan-driven material properties, making large-scale simulations more tractable. We modelled five glycans commonly found in the mucin glycoproteins, a protein known to be 50% - 80% glycosylated, and interacting with water to form hydrogels with several important physiological roles in health and disease. To compare water models, all simulations are performed using nanoscale molecular dynamics, with both an implicit (generalized born) and an explicit (transferable intermolecular potential-3) solvent model. We evaluated and optimized conformational properties such as flexibility profiles, dihedral distributions, puckering transitions, persistence length, and aggregation tendencies, all under different glycan densities and charge states. Improved implicit solvent model studies of glycan hydration forward the computational design of bioinspired materials. This progress allows for the development of tunable hydrogels, self-healing coatings, and protective bio barriers that accurately emulate the structural and functional features of natural glycoprotein networks.

Session IV: Materials for Health, Bioengineering and Society

Three-dimensional Printing of Alginate Scaffolds Crosslinked with Chitin, Chitosan, and the Chitin-glucan Complex Using Ethanol Solvent Exchange

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Abstract

This study investigates non-toxic, rapid crosslinking strategies for extrusion three-dimensional printing of sodium alginate scaffolds reinforced with mushroom-derived chitin–glucan complexes (CGCs). By combining alginate's shear-thinning, printable rheology with CGCs' higher flexibility and bioactivity vs crustacean chitin, composite inks aim to overcome alginate's weak mechanics and poor cell adhesion. We implement a solvent-exchange deposition modeling approach: the extruded filament encounters a locally controlled exchange medium that simultaneously removes a benign solvent and delivers crosslinking ions (e.g., calcium ion in aqueous microenvironments or buffered polymeric crosslinkers). This rapid, spatially confined gelation minimizes filament spreading, preserves high-resolution geometry, and enables stacked architectures with improved interlayer bonding. CGCs are dispersed or partially deacetylated to enhance intermolecular interactions with alginate, promoting hydrogen bonding and entanglement that raise stiffness and toughness without cytotoxic reagents. Outcome metrics include print fidelity, compressive and tensile modulus, viscoelastic recovery, porosity, and *in vitro* cell attachment/proliferation (mesenchymal stem cell and endothelial models). Anticipated benefits are mechanically robust, bio interactive scaffolds suitable for soft-tissue engineering and wound dressings, produced via a scalable, non-hazardous process. The work provides a pathway to translate mushroom-based polysaccharide reinforcements into clinically relevant, rapidly fabricated hydrogel constructs.

New Functionalized Scaffold Sensor for Advanced Stage Cancer Monitoring

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Abstract

Pancreatic cancer is increasingly prevalent, characterized by a high mortality rate. Due to the current limitations of diagnostic methods, the ability to detect this cancer in its early stages remains elusive, resulting in persistently low survival rates for individuals with pancreatic cancer. Nanomaterials are now getting more attention in the field of cancer research. Due to the unique properties, including high electrical conductivity, hydrophilicity, excellent thermal stability, large interlayer spacing, easily tunable structure, and high surface area, MXenes, a new and intriguing family of 2-dimensional transition metal carbides, nitrides, and carbon nitrides, have attracted a lot of interest in the field of nanomaterials. These nanomaterials are good at finding trace amounts of different analytes. Additionally, because of their tunable qualities, we can alter their structure and consequently shape their properties to meet the needs of sensing response. The smectite groups of natural clay minerals including montmorillonite (MMT) nanoclay, have the capacity to promote bone development and cell behaviour. In order to identify pancreatic cancer early, metal carbide MXene and their composites made with MMT nanoclay are showing promise in application of sensing response.

By observing the distinctive pattern in resistance change of these sensors, we can not only track their reaction but also tell cancerous samples apart from non-cancerous samples. Additionally, MXene's excellent selectivity aids in the identification of particular targeted analytes from a variety of different chemical and biological analytes, making them more trustworthy. The MXene-MMT composites-based scaffold sensor is anticipated to soon be able to both diagnose cancer and aid in tissue regeneration.

Simulating Glycan Barriers to Accelerate Therapeutic Delivery and Design

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[3]*Department of Physics, Northeastern University, Boston, USA*

Abstract

Effective therapeutic delivery requires navigating some of biology's most formidable molecular barriers - many of which are decorated or structured by glycans. My group develops computational and data-driven methods to understand and design around these glycan mediated challenges, spanning from viral immunology to therapeutic packaging and mucosal biology. At the viral interface, we have built a suite of modeling tools to characterize the dense glycan shields of pathogens such as human immunodeficiency virus and severe acute respiratory syndrome coronavirus-2. These simulations quantify how glycans mask protein surfaces and identify vulnerable sites that antibodies can exploit, offering guidance for immunogen design. Building on this, we integrate machine learning with molecular modelling to predict antibody-antigen binding interfaces, advancing both antibody engineering and our broader ability to design therapeutics that can selectively target glycosylated proteins. Beyond immunology, we apply these principles to therapeutic delivery. In collaboration with industry partners, we design glycopeptide-based polymers as bespoke packaging for nucleic acid therapies. By leveraging glycans and peptide motifs, these vehicles are engineered to penetrate mucus barriers, protect payloads, and enhance uptake efficiency. Complementing this, we use atomistic simulations of mucins, the heavily glycosylated polymers that form mucus hydrogels, to model drug-mucus interactions and understand how these networks regulate transport. Together, these efforts highlight how computation and data science can transform glycans from obstacles into design elements, enabling more effective strategies for drug delivery, gene therapy, and biomaterial innovation.

Novel Platinum Nanotherapeutics Induce Reactive Oxygen Species Storm to Combat Chemoresistant Cancers

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Abstract

Chemoresistance remains a critical challenge in effective cancer therapy. While reactive oxygen species (ROS) generation has emerged as a promising therapeutic strategy, current ROS-inducing agents often fail to achieve sufficient oxidative stress to eliminate resistant tumor cells. Here, we present carrier-platin, a novel platinum (Pt)-based nanotherapeutic engineered by uniformly confining ultrasmall Pt nanoparticles within a poly(amino acids) carrier. Carrier-platin rapidly induces a robust and sustained ROS burst in cancer cells, triggering cell death within just 30 min of treatment. Distinct from traditional Pt drugs like cisplatin that rely on DNA intercalation and apoptosis, carrier-platin operates through a non-canonical mechanism independent of DNA damage. This unique mechanism of action effectively bypasses key resistance pathways commonly upregulated in multidrug-resistant tumors. Carrier-platin exhibits broad-spectrum anti-tumor activity in multiple *in vitro* and *in vivo* murine cancer models—including those with established therapeutic resistance, while maintaining a favorable systemic toxicity profile. Our findings highlight a fundamentally new therapeutic mechanism of Pt-driven ROS catalysis that is

highly effective against chemoresistant cancer cells. By disrupting redox homeostasis beyond DNA repair, carrier-platin redefines the therapeutic potential of Pt-based agents and opens a new avenue for combating drug resistance in cancers.

A Molecular Blueprint for Mucin-inspired Biomaterial

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Abstract

Mucin inspired biomaterials represent a rapidly growing class of functional polymers engineered to replicate the selective permeability, lubrication, and molecular recognition properties of biological mucus. Mucin-2 (MUC2), the dominant mucin of the intestinal barrier, is an extreme case of this complexity exceeding 5,000 amino acids in length, with O-glycans comprising 40 - 80% of its total mass. This makes MUC2 extraordinarily difficult to study. Experimentally, its size and glycan heterogeneity confound structural characterization. We have built a scaled atomistic model of MUC2 that preserves its glycosylation patterns, domain architecture, and key physical properties. Using all-atom molecular dynamics simulations, we characterize its polymer behavior across three glycosylation states: unglycosylated, moderately glycosylated, and extensively glycosylated. We have determined the optimal model length and scale, and characterized chain extension, structural behavior, and interaction energetics as a function of glycan load. Glycosylation progressively expands the polymer chain through steric and electrostatic repulsion between O-glycan arrays. We further probe how this glycosylation dependent conformation controls the accessibility of sodium taurocholate, a major intestinal bile salt, along the polymer backbone. These results of chain extension and binding energetics provide a direct molecular basis for designing mucin inspired materials. Glycan density emerges as the primary lever over chain architecture and partitioning behavior. This work offers a principled, atomistically grounded framework for engineering glycopolymers for mucosal drug delivery, bioprotective coatings, and hydrogel scaffolds.

Session V: Functional, Sustainable and Next-Generation Materials

Metal Powder Preparation Using Gas Atomization Technology

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Abstract

Gas atomization technology is one of the most essential technologies for preparing metal powders. With this process, the liquid metal flowing from the melt delivery tube is atomized through a high velocity gas sprayed from a nozzle with an angled. In our work, the variation of the position of the melt delivery tube on the pressure at the tip of the delivery tube was investigated, and the effect of mass median diameter, particle size distribution, and yield was experimentally studied and analyzed. Clogging of the delivery tube was discussed. Experimental studies showed that the yield gradually increased at critical and prominence positions at low pressure and decreased at sag positions, providing significantly lower yields. At higher pressure, yields at critical and prominence positions gradually reduced, with prominence positions at 3 MPa producing powders with smaller average particle sizes and higher yields. With the increase in the length of the delivery tube, the flow resistance increased. Shortening the length of the tube reduces the flow resistance and increases the superheat of the melt.

Synthesis of Fe_xO_y/Activated Biochar Composite from Patchouli Biomass and Characterization of its Potency as Adsorbent of Organic Pollutant

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Abstract

Biochar is a porous material which can be produced by biomass waste pyrolysis and modified using metal oxide to improve its adsorption performance. Activated biochar (AB) was synthesized from patchouli biomass waste to study the effect of calcination temperature on its potency as a drug pollutant adsorbent. Research processes included the biomass pyrolysis with cobalt chloride activator, AB impregnation with ferric chloride ($FeCl_3$), $FeCl_3$/AB calcination at various temperatures, product characterizations (X-ray diffraction, fourier transform infrared (FTIR) spectroscopy), and paracetamol adsorption test at various concentrations. The paracetamol concentrations were analyzed using ultraviolet visible spectrophotometry. The adsorption data was treated using Langmuir, Freundlich, and Dubinin–Radushkevich (DR) models. The diffracto-grams indicated the α-Fe_2O_3, γ-Fe_2O_3, ferrosoferric oxide, and carbon turbostratic structures. The Fe_xO_y crystallinity increased by increasing temperature. The FTIR spectra significantly indicated the functional group changing at 600 °C. In the adsorption test, the Fe_xO_y/AB - 800 composite gave the highest adsorption capacity of 53.087 mg/g (Langmuir) with a correlation co-efficient of 0.964 (very high correlation), and the physical adsorption mechanism based on adsorption energy of 530.330 J/mol (DR) and 1/n value of 0.62 (Freundlich) provided the favorable adsorption based on both the separation factor R_L of 0.457 (Langmuir) and the n constant of 1.579 (Freundlich). Thus, the Fe_xO_y/AB - 800 composite has potential as an adsorbent of organic pollutants such as paracetamol.

Enhanced Power Conversion Efficiency and Stability of Copper Zinc Tin Sulfide Quantum Dot Based Photovoltaic Device by Incorporating Carbon Nanostructures in the Active Layer

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Abstract

A green and low temperature solvothermal have been adopted to prepare copper zinc tin sulfide (CZTS) quantum dots (QDs). The CZTS was used as light absorbing material in the photovoltaic device structure soda-lime glass/molybdenum/CZTS QDs (light absorbing layer)/cadmium sulfide/zinc oxide/aluminium to investigate its performance. Photovoltaic parameters obtained from the measurement are open circuit voltage (V_{oc}) of 0.67 V, short circuit current density (J_{sc}) of 15.8 mA/cm^2, a fill factor (FF) of 56.2%, and a power conversion efficiency (PCE) of 5.94% for active area of 0.5 ± 0.1 cm^2. CZTS QDs have lower mobility. If a material of higher mobility is added in CZTS, the performance of the photovoltaic device could be enhanced. In this regard, various allotropes of carbon has been incorporated in CZTS and investigated its photovoltaic performances. In case of reduced graphene oxide (rGO) incorporated CZTS QDs, the J_{sc} has been improved from 15.8 mA/cm^2 to 16.4 mA/cm^2, V_{oc} of 0.67 V, and FF of 56.7%. The PCE obtained for CZTS QDs-rGO hybrid device was 6.25%. The J_{sc} has been noticed to be improved even up-to 17.7 mA/cm^2 by adding conducting multi-walled carbon nanotubes (MWCNTs) to CZTS QDs. The CZTS QDs-MWCNTs hybrid device performance found to be enhanced with 6.77% PCE, V_{oc} of 0.67 V, and FF of 56.9%. In case of few layer graphene sheets incorporated CZTS QDs, the J_{sc} has been improved from 15.6 mA/cm^2 to 19.07 mA/cm^2, V_{oc} of 0.695 V, FF of 57.7%, and PCE of 7.64%. Improvement in performance of the CZTS based photovoltaic devices by incorporation of carbon nanostructures are attributed to the high electron/hole mobility, efficient light absorption, large exciton lifetime because of effective charge separation from QDs to carbon nanostructures, and fast charge transfer to current collector

Dual Emissive Carbon Dots for Sensing Applications

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Abstract

Carbon dots (CDs) have become increasingly popular in the past decade due to their unique optical properties, good biocompatibility, low toxicity, great aqueous stability, and facile synthesis. Our goal is to design and to develop fluorescent CDs with multiple emissions for sensing applications with improved sensitivity, selectivity and reliability. Two types of CDs will be presented for chemo-sensing applications. 1) Dual emissive CDs through a simple solvothermal method were obtained. The CDs showed excitation-dependent emission properties with both blue and green emissions as well as solvatochromic properties. Besides, the CDs' emissions could be affected by water in different organic solvents, which have been developed as efficient sensors for the detection of trace amounts of water. By taking advantage of the dual emissions, the ratiometric detection of water has been achieved. 2) CDs with multi emissions and chelating agents (dithizone) were developed to efficient detection of lead ions. Lead ions recovered fluorescence of CDs/dithizone complex solution efficiently. The enhancement of fluorescence could be developed for lead detection sensitively and selectively. In addition, by taking advantage of advanced data analysis such as principal components analysis, several metals could be differentiated utilizing changes of dual emissions.

Rare-earth-doped Nanostructured Phosphors in Recycled Glass Hosts: Sustainable Phosphor-in-glass Composites

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Abstract

Phosphor-in-glass (PiG) composites are increasingly explored in light emitting diode (LED) applications due to their enhanced durability and thermal resistance compared to traditional phosphors embedded in polymeric

resins, particularly under demanding operating conditions. A sustainable alternative involves embedding rare-earth-doped nanostructured phosphors into recycled silicate glass matrices. In this study, ceramic phosphors such as yttrium aluminium garnet (YAG) doped with europium (Eu^{3+}), dysprosium (Dy^{3+}), and samarium (Sm^{3+}), as well as Dy^3-doped zinc aluminate ($ZnAl_2O_4:Dy^{3+}$), were synthesized using a modified sol-gel method. Al, Y, Zn, Dy, Sm, and Eu nitrate salts were used as precursors and mixed with hexamethylenetetramine, which serves as the complexing agent. The reaction mixture was heated at 90 °C for 24 h in a sealed vessel, followed by drying at 200 °C and calcination between 900 - 1000 °C to obtain crystalline powders. Recycled glass was obtained by crushing commercial soda-lime bottles and milling the fragments to <44 μm. The phosphors were mixed with the glass powder and subjected to a brief thermal treatment at 800 °C for 10 min to form the composites. Structural (x-ray difraction), morphological (scanning electron microscope), and photoluminescence (PL) analyses were performed on the individual phosphors and the resulting PiG materials. To identify challenges and assess future perspectives, the PL behavior of the composites was evaluated under near-ultraviolet excitation using LED sources at 365 nm and 395 nm. This approach highlights the potential of combining luminescent nanomaterials with recycled waste to develop optical materials. The integration of rare-earth-doped phosphors into waste-derived glass hosts presents a promising route for utilizing sustainable raw materials in optoelectronic applications.

Session VI: Materials Design, Interfaces and Engineering Systems

Numerical Simulations and *In Situ* Investigations of Oxide Nanotube Arrays

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Abstract

Numerical simulations are widely used to predict the unique properties of materials. By systematically exploring a broad parameter space, they minimize the need for complex and resource-intensive experiments. More recently, emerging *in situ* experimental techniques have provided new opportunities to uncover novel material properties. Our *in situ* heating transmission electron microscopy studies of titania nanotube array architecture revealed the formation of a three-phase structure when pristine nanotubes were heated from room temperature to 950 °C. Molecular dynamics simulations demonstrated that high-energy ions can be channelled through the nanotubes and focused. This talk presents the methodology and key findings of these studies.

Exascale Transport Simulations for the Understanding of the Switching Mechanism in Atomically Thin Memristors

Liangbo Liang[1*], Wenchang Lu[2], Jameela Fatheema[3], Emil Briggs[2], Deji Akinwande[3], Jerzy Bernholc[2] and Panchapakesan Ganesh[1]

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Abstract

Non-volatile resistive switching (NVRS) has emerged as an important concept in the development of high-density information storage and computing. The recent discovery of NVRS in two-dimensional (2D) monolayer structures, such as molybdenum disulfide and hexagonal boron nitride (hBN), open a new avenue for memory/computing devices at the ultrathin scale. The fundamental switching mechanism in 2D monolayers, however, is not yet fully understood. It is hypothesized that vacancies in 2D monolayers mediate formation of filamentary channels leading to a high to low resistance state. However, questions remain as to why the current on/off ratio is strongly device-dependent and vary significantly among different experimental works. To address these questions, it is highly desirable to simulate the electronic transport in a realistic device geometry using ab initio approaches for comparison with experimental data. This is rather challenging as quantum transport simulations are computationally demanding. Here, for the first time, we carried out electronic transport simulations of systems consisting of a hBN monolayer sandwiched by top and bottom gold electrodes with the number of atoms up to 3,600. These large transport simulations are made possible by implementing the non-equilibrium Green's function method in a highly scalable first-principles density functional theory code: the real-space multiGrid that runs efficiently in the first exascale supercomputer, Frontier, at Oak Ridge National Laboratory. Systematic calculations reveal that experimental devices exhibit a wide range of on/off ratios (10^0 to 10^7) due to variations in interface distances between the electrode and hBN that significantly modulates the gold/hBN wavefunction overlap. Our work provides a deeper understanding of the resistive switching mechanism in atomically thin memristors and demonstrates the significance of interface distance in governing the current on/off ratio.

Two-way Shape Memory Polymers

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Abstract

Among shape memory polymers, two-way shape memory polymers — which can reversibly actuate in response to temperature changes — have attracted significant attention in recent years due to their broad potential applications, ranging from healthcare to aerospace. In this talk, I will present our research on two-way shape memory polymers conducted over the years, highlighting their use as artificial muscles, syntactic foams, and strain sensors. I will also discuss multifunctional two-way shape memory polymers, including those with properties such as three-dimensional printability, low creep, flame retardancy, and recyclability.

Surface Engineering Design for Medical Device Biocompatibility

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Abstract

Surface treatment plays a crucial role in improving the biocompatibility and bioactivity of medical devices. Bioactive surface treatments are applied to medical devices to improve their interaction with biological tissues. These treatments can promote desired biological responses such as cell adhesion, tissue integration, and reduced inflammation. Medical device manufacturers are often tasked with the arduous feat of developing new and improved materials to enhance the implant surface. This abstract provides an overview of various surface treatment techniques employed to enhance the performance of medical devices. Plasma spray coatings, such as Matrix HA® (hydroxyapatite) and Matrix Ti® (titanium), provide a biomimetic environment that encourages osseointegration and tissue regeneration. Surface modification techniques, including Matrix MCD® and Matrix Dual® texturing, alter surface topography using resorbable apatitic abrasive to promote cell attachment and tissue integration. Regulatory requirements and biocompatibility testing must be considered when developing and applying bioactive surface treatments to ensure the safety and efficacy of the devices. Collectively, these surface treatment approaches offer promising strategies to optimize medical devices for improved patient outcomes and enhanced medical interventions.

How to Build a "Bridge"? Nature's Strategy for Connecting Hard and Soft Materials

Benny Bar-On*

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Abstract

Load-bearing biological materials employ specialized bridging regions to connect material parts with substantially different mechanical properties (hard vs soft). While such bridging regions have been extensively observed in diverse biomaterial systems that evolved through distinctive evolutionary paths—including arthropod parts, dental tissues, and marine threads—their mechanical origins and functional roles remain vague. In my talk, I introduce a hypothesis that these bridging regions have primarily formed to minimize the near-interface stress effects between the connected material parts, preventing their splitting failure, and obtain a simple theoretical law for the optimal mechanical properties of such bridging regions. I demonstrate this principle through finite element simulations and physical experiments on a model synthetic-material system and verify its predictability for different biomaterial systems. The bridging principles of biological materials can be implemented into advanced material designs—paving the way to new forms of architected materials and composite structures with extreme load-bearing capabilities.

Thin-film Thickness Effects on the Optical Properties of Silver-aluminum alloy

Connor Lin, Ryan Lin and Guowen Ding*

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Abstract

Accurate refractive-index (RI) data are vital for developing novel optical applications, yet those RI of most thin-film metal alloys remain unknown and difficult to predict because they vary strongly (up to 100 times) with deposition conditions and film microstructure. Our laboratory published a model that uses RI ratios to reduce the influence of these factors and predicts the RI of silver alloys from pure silver data, alloy composition, and resistivity. However, the influence of film thickness on its predictive limits remains unquantified. This study evaluates the model's predictive accuracy for silver-aluminum (Ag-Al_x) alloy thin films deposited via magnetron sputtering across a varying range of deposition thicknesses. Our experimental data identifies a critical thickness threshold where the alloy's electrical and optical properties stabilize; below this threshold, on the thinner side, resistivity increases as the film becomes thinner, while beyond it, the resistivity remains generally flat, converging to a consistent bulk-like value. By mapping the correlation between film thickness, alloy concentration, and the resulting RI (n and k), we establish a predictive baseline for Ag-Al_x alloy applications that significantly improves upon the limitations of existing models. The results provide a more reliable basis for estimating the optical properties of Ag-Al_x alloy films and for designing optical coatings with controlled electrical and optical performance.

Zero Harm and Higher Efficiency: Readiness, Reception, and Control of Autonomous Haulage Systems in Mining

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Abstract

Autonomous Haulage Systems (AHS) are redefining surface mining operations by enhancing safety, improving efficiency, and minimizing human exposure to hazardous environments. This paper investigates the industry's readiness for AHS adoption, evaluates the reception of these systems by operators, supervisors, and stakeholders, and analyses the technological and operational control mechanisms that support AHS deployment. Through a synthesis of case studies and recent implementations, the study outlines safety improvements, productivity gains, and cost optimization enabled by AHS. It also addresses key challenges, including infrastructure requirements, change management, regulatory compliance, and interoperability. The findings underscore AHS as a strategic enabler of zero harm and sustainable mining performance.

Poster Session

Investigation of Mechanical Performance in Different Metal Additive Manufacturing Processes

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Abstract

Metal additive manufacturing (AM) fabricates metal components through a layer-by-layer deposition process. Compared with conventional machining or casting methods, AM offers several advantages, including greater design flexibility, improved material utilization, and rapid manufacturing capabilities. Consequently, it enables the production of complex structures that are difficult to achieve using traditional subtractive metal manufacturing techniques. In recent years, metal AM has been widely applied in aerospace, medical and biomedical engineering, and automotive industries. However, during the metal AM process, process parameters have a direct influence on melt pool stability and the quality of the fabricated parts. Improper parameter selection may result in defects such as porosity, lack-of-fusion defects, and microcracks in the printed components. These defects can significantly reduce the mechanical strength and fatigue life of the parts, particularly in high-strength alloys and stainless steel materials. Among stainless steels, 420 stainless steel exhibits good hardness, excellent wear resistance, and moderate corrosion resistance. Therefore, it has been widely used in molds and various industrial components. In this study, tensile specimens of 420 stainless steel were fabricated using different process parameters to evaluate the resulting mechanical properties. The experimental results indicate that when the laser power was set to 300 ± 50 W, the laser scanning speed to 800 ± 50 mm/s, and the hatch spacing to 100 μm, the printed parts demonstrated improved densification and enhanced tensile strength.

Overcoming Analytical Barriers in Dense Oxides: High-resolution Chemical and Dopant Mapping of Cerium-doped Multi-layer Garnet Films by Gallium Focused Ion Beam Time-of-flight Secondary Ion Mass Spectrometry

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Abstract

We report the detection and spatial mapping of dopant-related secondary ion signals in single-crystalline cerium (Ce^+)-doped lutetium aluminum garnet ($Lu_3Al_5O_{12}$:Ce, LuAG:Ce) films grown by liquid-phase epitaxy, using gallium ion (Ga^+) focused ion beam time-of-flight secondary ion mass spectrometry (FIB-TOF-SIMS). LuAG:Ce is a dense garnet oxide used in scintillation, phosphor, and laser devices, where nanoscale dopant distribution influences optical performance. Its high resistivity, chemical complexity, and sputtering resistance make nanoscale dopant analysis challenging. Under Ga^+ primary ion bombardment, we obtained clear secondary ion signals from the garnet matrix, including Ce^+, Lu^+, and oxide fragments (e.g., CeO^+, LuO^+). Sub-micrometer spatial resolution revealed relative dopant variations at growth-related features and interfaces without conductive coatings or extensive surface preparation. Local Ga implantation reduced charging sufficiently for stable image acquisition while preserving matrix-specific spectral features. These results establish Ga^+ FIB-TOF-SIMS as a viable method for high-resolution dopant mapping and microstructural characterization in thick epitaxial oxide films, complementing electron microscopy in the study of garnet-based photonic and scintillation materials.

Process for Preparing Yttrium Disilicate Coating Using Sol-gel Solution and Oxyacetylene Flame

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Abstract

This study focuses on the use of oxyacetylene flame thermal spraying with external injection of a sol-gel solution as a novel alternative for synthesizing yttrium silicate ($Y_2Si_2O_7$) crystalline phases. Sol-gel solutions with different molar concentrations of yttrium (Y)/silicon (Si) precursors were injected into the flame to obtain a coating on an Inconel 718 substrate. The results showed that a 1:1 Y/Si precursor ratio in the solution promoted the formation of $Y_2Si_2O_7$ scale, while a 5:5 Y/Si precursor ratio in the solution promoted a dense, low-porosity coating, but with the presence of microcracks on the substrate surface. This coating was composed of $Y_2Si_2O_7$ with a monoclinic crystalline phase $Y_2Si_2O_7$, along with other secondary crystalline phases of nickel-chromium alloy, nickel oxide, and chromium. All these findings support that a flame temperature of 2300 °C in the oxyacetylene flame thermal spraying process is the temperature required for sol-gel phase synthesis.

Hydrogen-induced Defect Formation in Yttrium-based Coatings for Dry Etching Processes

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Abstract

As the critical dimensions of semiconductor devices shrink, especially for the sub-3 nm node, dry etching processes increasingly employ complex hydrogen-containing plasma mixtures to achieve precise pattern control. Hydrogen plasma exposure can induce degradation of chamber coatings and the formation of yttrium-based particle defects, resulting in significant yield loss. This study investigates the material properties and microstructural design strategies of yttrium-based coatings to enhance hydrogen resistance and process stability. Hydrogen-induced defect formation was modelled as a function of materials phase and deposition conditions, and correlations between microstructural characteristics and plasma-induced degradation were evaluated. From a materials perspective, yttrium(III) oxide (Y_2O_3) and yttrium aluminum garnet (YAG) coatings were experimentally assessed. Regarding deposition methods, commonly employed plasma-resistant coating techniques, including plasma spraying, aerosol deposition (AD), and physical vapor deposition (PVD), were systematically reviewed. Exposure to hydrogen-rich plasma revealed hydroxide formation, approximately 20 nm in thickness, on Y_2O_3 grains, while no transformation to a new crystalline phase was observed on YAG grains, as confirmed by crystallographic analysis. Concurrently, microstructural evaluation demonstrated that PVD coatings minimize pores and reactive species diffusion paths, effectively mitigating plasma-induced degradation. These observations confirm that PVD YAG is a promising candidate for suppressing hydrogen-induced particle formation and enhancing the durability of etch chamber components in sub-3 nm node dry etching processes. The results provide a mechanistic understanding of hydrogen plasma-coating interactions and strategies for the optimized design of plasma-resistant chamber coatings.

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