36th Annual PNWAVS Symposium

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Abstract Book

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Plenary Talk

Thursday, August 28, 7:30 PM: **A Surface Scientist's Journey from Single Crystals to Biomaterials**

David Castner
University of Washington

Surface science plays an important role in research and development areas such as catalysis, biomaterials, microelectronics, clean energy and corrosion. The toolbox of surface scientist allows us to move across research topics and make significant impacts in both industrial and academic settings. The typical surface scientist is an expert in multiple techniques, surface modification, sample preparation/handling and instrumentation. We have all benefited from the significant advances that have occurred in the past 50 years in improved instrumentation, introduction of new techniques and development of sophisticated data analysis methods, which has allowed us to perform detailed analysis of increasing complex samples. For example, comprehensive analysis of surfaces and surface immobilized molecules with modern surface science instrumentation provides an unprecedented level of detail about the immobilization process and the structure of the immobilized molecules. Results from XPS, ToF-SIMS, NEXAFS, SPR and QCM-D, AFM, and SFG vibrational spectroscopy combined with computation methods provide important information about surface chemistry and structure. However, even with the advances that

have been achieved with these powerful surface science techniques, there remain many significant challenges for surface scientist. These include characterizing the surface chemistry and structure of nanoparticles, determining the atomic level structure of complex molecules bound to surfaces, 3D imaging of samples, and improved sample preparation methods that maintain materials in a relevant state when using UHV-based analysis techniques.

I will discuss my journey from small molecule chemisorption and reactivity studies on single crystal surfaces followed by industrial catalysis research and eventually moving to biomedical surface analysis."

Thursday, August 28, 8:30 AM: **New opportunities with defects in superconducting qubits**

Mo Chen
University of Washington

Superconducting qubits are among the leading platforms for realizing fault-tolerant quantum computation. However, atomic-scale material defects, known as two-level systems (TLS), naturally occur at the surfaces and interfaces of all materials that constitute superconducting qubits. These TLS defects limit the performance of superconducting qubits, affecting both the coherence of individual physical qubits, and the optimization landscape of large-scale quantum processors. In this talk, I will present a new approach that directly modifies the properties of TLS through nanoscale engineering. This transforms TLS into a potentially useful quantum resource, opening new opportunities in the superconducting qubit platform.

Thursday, August 28, 9:30 AM: **Electron Ptychography: Using Computational Lenses to Probe Quantum Materials**

Kayla Nguyen
University of Oregon

Electrons play a pivotal role in stabilizing matter, but they are also tools that can reveal the underlying physics of complex systems from high energy physics to condensed matter. Electrons can be used as imaging probes, where properties of matter such as ferroelectricity, magnetism or topology can be observed atom-by-atom. In this talk, I will discuss a new type of electron probe which can image magnetism and chiral order of topological structures such as magnetic skyrmions. I will also show how electron ptychography, an iterative computation imaging technique, can improve resolution beyond the numerical aperture of the electromagnetic lenses to the sub-angstrom limit in a conventional electron microscope. Using this technique, we essentially develop a 'computation lens' approach to imaging, opening opportunities to explore new physics in emergent materials beyond physical lenses in a cost-effective manner, and thus expanding access to high-resolution imaging approaches to a broader range of institutions.

Thursday, August 28, 10:30 AM: **High-Throughput Screening of Molecular Layer Deposition Processes for EUV Photolithography**

David Bergsman
University of Washington

Because of its ability to deposit organic, inorganic, and hybrid ultrathin films with sub-nanometer thickness and compositional control, molecular layer deposition (MLD) has seen growing interest for use in technologies where precise interfacial control is essential, such as in semiconductor processing, membrane separations, and catalysis. However, development of these technologies is inhibited by the relatively slow process times for MLD vs atomic layer deposition and the large number of combinations of inorganic & organic reactants available to MLD. This presentation will highlight the intrinsic advantages of accelerating MLD process development, both for technology development and for fundamental research. First, an approach for rapidly screening new materials deposited by MLD using a custom-built, high-throughput, multiplexing MLD-style reactor will be discussed. In such a system, multiple reaction chambers are connected to shared reactants and pumping lines, allowing for the elimination of redundant reactor components and reducing capital costs compared to an equivalent number of independent systems. Then, several examples of how this approach can be applied to future technologies, such as EUV photolithography, will be given, demonstrating how materials made using these parallel systems can be screened for their properties of interest and be used to obtain process-structure-property relationships.

Thursday, August 28, 1:20 PM: **Nanosecond electron microscopy of electrically triggered material dynamics**

Daniel Durham
Argonne National Laboratory

Electrically controlled material responses at nanosecond speeds (e.g. piezoelectric, ferroelectric, phase transitions, electrochemical) are important for modern and next-generation electronics, especially in the GHz regime. Determining the underlying nanoscopic mechanisms and their rate-limiting steps is important to understand and ultimately improve high frequency electronic properties. I will introduce voltage-triggered ultrafast electron microscopy at Argonne National Laboratory, which allows to directly image reversible, electrically stimulated dynamics with nanometer-nanosecond resolution [1,2]. As a first demonstration, we addressed the electrical pulse switching mechanism of room

temperature charge density waves in 1T-TaS2 [1]. Diffraction was used to track the atomic structure dynamics, while imaging revealed heterogeneous strain dynamics. We found that two processes contribute to charge density wave melting on nanosecond scales: electrical heating and acoustic resonance. We anticipate that this approach will provide key insights into the dynamics of a broad range of electronic materials and interfaces.

[1] DB Durham & TE Gage et al. "Nanosecond Structural Dynamics during Electrical Melting of Charge Density Waves in 1T–TaS2." Phys. Rev. Lett. 2024.
[2] TE Gage & DB Durham et al. "Nanosecond Electron Imaging of Transient Electric Fields and Material Response." ArXiv:2306.01171. 2023.

Friday, August 29, 8:00 AM: **What can simulations teach us about interlayer heterogeneity in covalent organic frameworks?**

Tim Kowalczyk
Western Washington University

Two-dimensional covalent organic frameworks (COFs) are porous materials consisting of intermolecularly bound, atomically thin layers of organic linker and spacer precursors. COFs provide a synthetically tunable platform for the design of surfaces and interfaces that can facilitate a variety of valuable catalytic and electronic processes. Post-synthetic or one-pot functionalization of COFs creates opportunities to introduce heterogeneity across neighboring layers of the material;[1] however, many low-energy heterogeneous configurations are possible, and traditional characterization methods can struggle to distinguish among them. Drawing from examples encountered over the course of a decade's exploration of COFs as candidate materials for singlet fission,[2] here we discuss how electronic structure simulations can help to close the loop from synthesis and characterization to design principles for heterogeneously layered 2D COFs with targeted photophysical and electronic properties. Consequences of interlayer heterogeneity and pore-filling for photoexcitation and electron transfer within the framework will be emphasized.[3]

(1) Frey, L. et al. Angew. Chem. Int. Ed. 2023, 62, e202302872.
(2) Laszlo, V.; Kowalczyk, T. J. Mater. Chem. A 2016, 4, 10500.

(3) Leo, T. M. et al. J. Chem. Phys. 2024, 160, 184704."

Friday, August 29, 10:20 AM: **Atomic Scale Understanding of Material Synthesis and Degradation Mechanisms: Two Sides of the Same Coin**

Arun Devaraj, Venkata Bhuvaneswari Vukkum, Jack Grimm, Semanti Mukhopadhyay, Francelia Sanchez Escobar, Tingkun Liu and Harilal Sivanandan
Pacific Northwest National Laboratory

Materials scientists dream of pinpointing each atom's location to unlock how processing affects material properties. Such atomic-level insights can pioneer new processing techniques, like solid-phase deformation and additive manufacturing, leading to groundbreaking materials. This knowledge is equally crucial for researchers studying how atoms shift under extreme conditions like corrosion, neutron irradiation in nuclear reactors, or hydrogen exposure. This understanding helps design durable, high-performance materials for applications in extreme environments. Given the complexity of the atomic movements during both material synthesis and material degradation, no single method can cover details from the atomic to the component scale. Hence, a blend of in situ and ex situ characterizations, computational simulations, and mechanical testing is necessary. This talk will showcase our multidisciplinary efforts in tackling these challenges, leveraging cutting-edge microstructural characterization methods, including advanced electron microscopy, in situ and cryogenic atom probe tomography (APT), and synchrotron-based high-energy X-ray diffraction. Coupled with predictive modeling and mechanical testing, these techniques enable us to bridge fundamental scientific understanding with applied innovations in material synthesis and degradation. Together, these advances provide critical insights to enable the next generation of materials for diverse applications.

General Talks

Thursday, August 28, 9:10 AM: **Defects and disorder in superconducting qubits: mechanisms of Ta oxidation and strategies for oxidation suppression**

Peter Sushko
Pacific Northwest National Laboratory
Aswin kumar Anbalagan, Chenyu Zhou, Junsik Mun
Brookhaven National Laboratory
Conan Weiland
National Institute of Standards and Technology
Yimei Zhu, Mingzhao Liu , Andrew L. Walter , Andi M. Barbour
Brookhaven National Laboratory

Coherence times of superconducting qubits can be affected by the defects and disorder at the interfaces of the superconducting components. For example, spontaneous oxidation of Ta and Nb results in the formation of suboxide phases and surface amorphization that contribute to dielectric losses within such native oxide layers. Mitigating undesirable effects of surface oxidation requires understanding the mechanisms of interfacial interactions at the atomic scale. We will review recent experimental studies that provide new insights into the atomic structure and composition of the native oxide layer and focus on the atomic-scale mechanisms of Ta surface modification due to their interaction with oxygen and other metal species. In particular, we consider energetics and pathways of the early stages of the Ta(110) surface oxidation, including propagation of the oxidation front into the Ta subsurface and corresponding electronic structure changes. We also explore strategies for suppressing Ta oxidation with the help of reactive metal coating and noble metal alloys. Our studies highlight the need to understand better the initial stages of oxidation and, more broadly, chemical modification of superconducting surfaces and disorder resulting from these processes and to design scalable approaches for mitigating the effects of disorder.

Thursday, August 28, 11:10 AM: **Tuning surface structural and electronic properties of high entropy oxide thin films for water oxidation**

Le Wang, Minju Choi, Krishna Prasad Koirala, Mark Bowden
Pacific Northwest National Laboratory
Dongchen Qi
Queensland University of Technology
Anton Tadich
Australian Synchrotron
Hsin-Mei Kao
Oregon State University
Zihua Zhu, Yingge Du
Pacific Northwest National Laboratory

High-entropy oxides (HEOs) offer exceptional compositional flexibility and structural stability, making them promising materials for energy and catalytic applications. In this work, we investigate the impact of oxygen vacancies on the lattice structural, electronic, and electrochemical properties of epitaxial La(5B)O3 thin films, where 5B=Cr0.2Mn0.2Fe0.2Co0.2Ni0.2, synthesized by pulsed laser deposition (PLD). By systematically varying the oxygen partial pressure (PO2) during growth, we tune the oxygen vacancy concentration and investigate its influence on lattice structure, charge distribution, and surface oxygen evolution reaction activity. Comprehensive characterizations, including X-ray diffraction, scanning transmission electron microscopy, X-ray absorption spectroscopy, electrochemical measurements, and time-of-flight secondary ion mass spectrometry reveal a strong correlation between surface composition, defects, and water oxidation activity/stability. These insights will enable rational navigation of the vast configurational space in multicomponent systems, ultimately guiding the design and synthesis of robust, functionally adaptive
materials for electrocatalysis.

Thursday, August 28, 11:30 AM: **Molecular Packing Modulates Charge–Exciton Dynamics in Organic Solar Cells Based on Non-Fused Ring Acceptors**

Qian-Qian Zhang and David Ginger
Department of Chemistry, University of Washington

The advancement of high-efficiency and cost-effective organic solar cells go hand in hand with leaps in fundamental understanding. In the case of non-fused ring acceptors, further

understanding of how solid-state structure modulates key photo-physical processes is crucial for enabling such advancements. In this study, we elucidate the role of molecular packing in exciton and charge dynamics by systematically investigating a series of L-type acceptors with progressively extended side chains. Subtle variations in side-chain architecture leads to pronounced differences in molecular packing at the single-crystal level and these structural motifs persist upon film formation, as confirmed by GIWAXS. These packing configurations substantially affect both exciton delocalization and the charge-transfer (CT) character of the initial excited state. Here, using electroabsorption spectroscopy, we show that the L2-C11 derivative—with its three-dimensional packing framework—exhibits the largest dipole moment response and the strongest CT character. Further, with transient absorption spectroscopy, we observe that face-on oriented films (L2-C11 and L2-C9) show clear signatures of non-geminate recombination, suggesting that orientation plays a critical role in charge-exciton interactions at molecular interfaces. Collectively, our findings underscore the high sensitivity of exciton and charge dynamics to solid-state packing and provide mechanistic insight into structure–function relationships in non-fused ring acceptor systems.

Thursday, August 28, 11:50 AM: **High-Throughput MLD Screening of Photoresists for EUV Lithography via UV and E-Beam Exposure**

Duncan Reece
University of Washington
Emily Crum,
Columbia University
Jane Keth and David Bergsman
University of Washington

As semiconductor patterning approaches sub-5 nm features, next-generation photoresists must deliver high resolution, stability, and compatibility with extreme ultraviolet (EUV) lithography. Current EUV photoresist materials face challenges including deposition ease and sub-nanometer chemical uniformity. Molecular layer deposition (MLD) offers precise control over thin-film structure and composition, enabling tailored hybrid materials to address these challenges. Using a custom high-throughput multi-chamber MLD system, we synthesized 18 organic-inorganic hybrid films from two organometallic precursors (trimethylaluminum/diethylzinc and tetrakis(dimethylamino)tin(IV)) paired with six organic linkers. While previous work demonstrated MLD-based EUV photoresists with aluminum and tin, the organic reactant's influence on photoresist properties remains underexplored.

Films were screened for growth rate, deposition ease, uniformity, and ambient stability. Photochemical reactivity was assessed by measuring thickness changes before and after solvent exposure, with and without deep UV treatment. High-performing films underwent electron beam lithography as an EUV surrogate, followed by development to evaluate feature resolution and pattern fidelity using scanning electron microscopy and profilometry. Mechanical durability was tested via nanoindentation, while chemical transformations were characterized using FTIR and XPS. Results identified material systems combining robust environmental and chemical resistance with promising lithographic performance and photo-reactive behavior. While EUV lithography remains the ultimate target, e-beam serves as a high-resolution surrogate for photoresist development. This integrated approach demonstrates high-throughput MLD's power combined with multi-parameter screening for accelerating advanced material discovery for next-generation lithographic technologies.

Thursday, August 28, 2:00 PM: **Investigations with a Prototype Hydrogen Focused Ion Beam Instrument**

Chad Rue
Thermo Fisher Scientific

A plasma FIB instrument has been modified to enable operation with hydrogen as the source gas. Plasma composition, FIB performance specifications, and experimental considerations are discussed. The instrument can be used to deliver precise doses of hydrogen ions with high spatial resolution, so specific microstructural features can be targeted. Because it is based on a DualBeam FIB/SEM platform, the user may perform in-situ SEM imaging of the sample during the hydrogen delivery. An additional advantage of this instrument is that the FIB can revert to conventional source gases (Xe, Ar, O_2, or N_2) to perform routine FIB analyses (cross sectioning, TEM lamella prep, APT sample prep) after the hydrogen irradiation step. Thus, hydrogen exposure and subsequent analysis can be performed in the same tool session, without venting cycles or the need to move the sample between tools.
 The hydrogen plasma produces three different hydrogen ion species (H^+, H_2^+, and H_3^+). An optional magnetic dispersion mode allows the user to spatially separate the ions and observe their behaviors independently. Irradiation with hydrogen ion beams creates an array of interesting embrittlement and corrosion effects on samples, including blisters, cracks, sub-surface porosity, and hydride formation. Results are shown for titanium, zirconium, aluminum, steel and stainless-steel alloys. Possibilities for site-specific hydrogen implantation and chemical reduction are also discussed.

Thursday, August 28, 2:20 PM: **ToF-SIMS, a unique tool in critical minerals and materials research**

Zihua Zhu, Xin Zhang, Yingge Du and Hsin-Mei Kao
Pacific Northwest National Laboratory

Critical minerals and materials research has been increasingly interesting in the last several years. Compared to popularly used material characterization tools, such as scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS), time-of-flight secondary ion mass spectrometry (ToF-SIMS) can play a unique role in their characterization due to several distinct advantages. The first advantage is ToF-SIMS' excellent sensitivity. Detection limits in the parts per million (ppm) range are easily achievable with ToF-SIMS, offering sensitivity 2-3 orders of magnitude higher than that of XPS or SEM/TEM-EDX. Such an advantage is particularly useful in detecting rare earth elements, whose concentrations are normally at the ppm level. The second advantage is that the ToF-SIMS spectra can provide valuable information to distinguish single atom adsorption from cluster adsorption on a substrate, which is highly interesting in the study of single atom catalysis. In addition, differentiating surface adsorption, bulk doping and phase mixing states are highly valuable for mineral studies, and ToF-SIMS can readily achieve this. Furthermore, ToF-SIMS is sensitive to the detection of light elements such as H, Li, and B. In this presentation, several examples from my lab will be used to demonstrate the advantages of ToF-SIMS. Our observations indicate that ToF-SIMS can play a significant role in the characterization of critical minerals and materials.

Thursday, August 28, 2:40 PM: **Imaging ToF-SIMS analysis of tumor microenvironments**

Lara Gamble
University of Washington

Cell growth regulation, metastatic potential, and drug resistance are associated with the tumor microenvironments. Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is a sub-micron spatial resolution imaging mass spectrometry technique used for chemical imaging. We use a combination of ToF-SIMS and H&E staining to analyze mouse pancreatic tissue slices by imaging tumors in a pIns-MycERTAM/p53-/- mouse model. TOF-SIMS was performed with an ION-TOF TOF.SIMS 5-100 instrument (ION-TOF GmbH, Münster, Germany) equipped with a liquid metal ion gun (LMIG) for analysis and an electron flood gun for charge neutralization.   Our analyses of the pIns-MycERTAM;p53−/− tumor microenvironment has identified and mapped molecules that play key roles in tumor metabolism including nucleic

acids, organic acids and lipids, as well as inorganic ions. We provide evidence of significant metabolic change occurring within Myc-driven β cell tumors and surrounding stromal region over a 12-day period and demonstrate that TOF-SIMS imaging is a useful tool for spatial characterization of metabolite changes in the Myc model. Our analyses provide evidence that significant metabolic changes occur in the tumor microenvironment in response to Myc activation and that the metabolic profiles of the tumor and the stroma differ dramatically.

Thursday, August 28, 3:30 PM: **Embedding sustainability into early-stage materials research: UW's LCA platform and an e-waste case study**

Rachel Woods-Robinson
Clean Energy Institute, University of Washington

Research and innovation in materials science often aim to advance global sustainability and societal well-being. However, quantitative sustainability metrics are rarely included early in the materials design process, likely due to disconnects between materials science and sustainability fields. Life Cycle Assessment (LCA)—which quantifies impacts from raw material extraction to end-of-life—can help guide low-environmental-impact solutions, circular strategies, and reduced harm to people and communities. However, LCA is usually performed only after scale-up to high technology readiness levels (TRLs), once it is difficult to make design changes. This risks "technology lock-in," where early unexamined choices risk becoming entrenched. To address this gap and promote sustainable design from the outset, UW's Washington Clean Energy Testbeds (WCET) has launched a new LCA service for researchers and industry developing low-TRL clean technologies. Here, we demonstrate the approach through an early-stage startup developing a novel leaching and nano-filtration process for recovering critical metals from electronic waste. In this case study, iterative LCA identified highest-impact steps, guided greener substitutions, and help lead to 5x lower GHG emissions than incumbent methods. We demonstrate how proactive, early-stage LCA can de-risk technology pathways, improve environmental performance, and give innovators a competitive edge by embedding sustainability into design from the start.

Thursday, August 28, 3:50 PM: **Revisiting Efficiency Limits in Si-Perovskite Tandem Solar Cells—Pushing Theoretical Boundaries through modelling**

Akash Dasgupta
University of Washington
Henry Snaith,
University of Oxford

The efficiency of Si-perovskite tandem solar cells has rapidly improved over the past decade, with record performances now surpassing the once-predicted 32% limit. In this study, we revisit efficiency ceilings by incorporating new ellipsometry data to obtain accurate optical constants and by considering advances in the radiative efficiency of the perovskite top cell. Earlier estimates relied on conservative assumptions of material quality and optical losses, but recent progress in single-junction perovskites suggests further gains are achievable. By systematically simulating a broad range of perovskite bandgaps and radiative efficiencies, we show that efficiencies approaching 36% are possible if tandem sub-cells can match the performance of today's high-efficiency single-junction devices. Notably, improving the perovskite layer's radiative efficiency to 10% yields substantial gains, while in the radiative limit, efficiencies up to 38% are predicted. These projections, which exceed current records, establish a "future-proofed" maximum PCE and highlight the importance of optimizing radiative efficiency and ideality factor in tandem architectures. Our study also updates prior benchmarks by introducing a library of ellipsometry-derived optical constants for use in device modeling. This dataset enables more accurate simulations and refined analysis of light management strategies in tandem cells. The findings underscore the potential for further efficiency gains in Si-perovskite tandems and outline a roadmap for future research. By identifying key opportunities in material quality, radiative efficiency, and light-trapping techniques, we set the stage for the next generation of high-performance tandem solar technologies.

Thursday, August 28, 4:10 PM: **Optical property and hygroscopicity of solid strongly absorptive brown carbon in wildfire smoke**

Zezhen Cheng, Amna Ijaz, Manish Shrivastava
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Daniel Veghte,
OSU
Gregory Vandergrift,
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Kuo-Pin Tseng,
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Will Kew
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Kaitlyn Suski
Rainmaker Technology Corporation
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Wildfires emit solid-state strongly absorptive brown carbon (solid S-BrC, commonly known as tar ball), critical to Earth's radiation budget and climate, but their highly variable light absorption properties are typically not accounted for in climate models. Literature reported solid S-BrC optical properties are highly variable, leading to significant uncertainties about their direct climate effects. Moreover, the interaction between solid S-BrC and clouds is typically neglected due to the common belief that they are hydrophobic. Here, we investigate the physicochemical and optical properties of solid S-BrC collected from the Pacific Northwest wildfire in September 2017, where more than 90% of particles are solid S-BrC with a measured refractive index at 550 nm wavelength equal to $1.49+0.059i$. Furthermore, we found that ~50% of solid S-BrC particles are hydrophilic and can form core-shell morphology at 5 °C and > 97% RH, possibly due to a highly oxygenated surface layer, making them potential cloud condensation nuclei. This core-shell morphology could enhance their absorption cross-section at 550 nm by a factor of 2 due to the lensing effect. In addition, SEM images show that at least 1% solid S-BrC has organic coatings, which leads to higher lensing enhancement than water coating. We conclude that more studies are necessary for models to improve the parametrization of the light-absorption properties of wildfire aerosol to

incorporate the contribution of solid S-BrC and their interactions with water to predict Earth's radiation budget accurately.

Friday, August 29, 8:40 AM: **Understanding of MOF Electrocatalytic Stability via In-situ Characterization**

Qiaowan Chang
Washington state university

Mechanistic   Metal–organic frameworks (MOFs) have emerged as promising candidates in electrocatalysis, particularly for the electrochemical reduction of carbon dioxide (CO2RR). Despite advances in enhancing catalytic activity and selectivity, the long-term electrocatalytic stability of MOFs remains insufficiently understood. In this study, we examine the stability and structural evolution of Zn-ZIF-8, a prototypical MOF catalyst, under CO2RR conditions. Using both batch and flow cell configurations, we assessed catalytic performance over time and observed that stability is strongly dependent on the applied electrochemical potentials. To elucidate degradation mechanisms, we conducted in-situ X-ray absorption near-edge structure (XANES) and in-situ X-ray diffraction (XRD) analyses. In-situ XANES revealed evolutions in the Zn–N4 coordination environment of the active sites, while in-situ XRD indicated bulk transformations in the long-range crystalline structure of Zn-ZIF-8 during electrolysis. These findings provide critical mechanistic insights into the structural dynamics governing MOF catalyst stability and inform the rational design of more durable MOF-based electrocatalysts for CO2RR applications.

Friday, August 29, 9:00 AM: **Tuning Catalytic Reactivity via Wetting Control Through Oxygen Vacancies: Ru Clusters, TiO2 and CeO2 Supports**

Carrington Moore, Jean-Sabin McEwen and Charles Umhey
Washington State University
Linxiao Chen,
University of North Texas

Hydrogenolysis is a process that can be used to upcycle polyolefins into usable materials. The rampant amount of plastics that have infiltrated the waterways are such polyolefins and motivates the need for a divergence and processing of end waste. Ru nanoparticles on a CeO2 support have already been identified as optimal for hydrogenolysis however it was unclear the structure of the particles on the surface. The Ru nanoparticles on the CeO2 surface are found to flatten, or wet the surface, and that results in increased activity. The

metal-support interaction that leads to the wetting and the size-dependency of the nanoparticles is poorly understood. In testing the wetting behavior, the Ru nanoparticles were adsorbed on reducible oxides, the known support CeO2, and anatase TiO2. In the coverage range of 0.06-0.98 Ru nm-2 it was found that TiO2-A does not wet the surface. However, at low coverages of less than 0.25 Ru nm-2 CeO2 was found to have flat structures. The difference between these two supports is attributed to the naturally forming subsurface oxygen vacancies in CeO2 (0.25 ML) [1]. When the CeO2 surface was modeled computationally without the oxygen vacancies the nanoparticles remained clustered and did not flatten as was seen with the oxygen vacancy surface. Thorough categorization and experimental and computational investigation of the surface highlights the importance of oxygen vacancies in the supports for wetting of clusters on the surface.

[1] Linxiao Chen, Carrington Moore, Charles Umhey et al., Journal of the American Chemical Society (submitted).

Friday, August 29, 9:20 AM: **Influence of pre-adsorbed hydrogen on platinum on the adsorption enthalpies of solvent molecules**

Valeria Chesnyak
Oregon State University/ Pacific Northwest National Laboratory
Arjan Saha,   Marcus Sharp
Pacific Northwest National Laboratory
Nida Janulaitis
University of Washington
Zbynek Novotny,
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Charles T. Campbell
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Líney Árnadóttir
Oregon State University

Understanding how the presence of different species affects the adsorption enthalpies on catalytic metal surfaces is essential for heterogeneous catalysis and electrocatalysis. While adsorption energies of small reactants on metal catalysts in vacuum have been reported, the impact of coadsorbates remains poorly understood. Computational methods such as density functional theory (DFT) can predict trends of adsorption energetics, including coadsorption effects at the catalyst interface. However, these models require experimental

benchmarks for validation, as significant discrepancies persist between calculated and experimental adsorption enthalpies. We present here results aimed at providing benchmarks for co-adsorptions and the effect of co-adsorbates on the adsorption enthalpies. Single Crystal Adsorption Calorimetry (SCAC) is capable of directly measuring the molecular and dissociative adsorption enthalpies on well-ordered single crystalline surfaces. We employ a state-of-the-art microcalorimeter to understand coadsorption-induced effects of common agents in catalysis on surfaces. Differential heats of adsorption for water and methanol on hydrogen-covered Pt(111) are reported. Molecular hydrogen dissociates on Pt(111) to form a hydrogen atom adlayer at cryogenic temperatures (100 K) and drastically reduces the heat of adsorption of the solvent molecules. Furthermore, differences between adsorption enthalpies at 100K vs. 130K suggest different growth dynamics on hydrogen-precovered surfaces. Understanding the effects of hydrogen coverage on the adsorption energies of solvent molecules provides important benchmarks for validating computational models.

Friday, August 29, 9:40 AM: **Ethanol Oxidation over Single-atom Model Rh/Fe3O4(001) Catalysts**

Daniel Baranowski, Marcus A. Sharp, Zbynek Novotny, Bruce D. Kay, Zdenek Dohnálek
Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory

The selective oxidation of alcohols like ethanol, a renewable feedstock, is of pivotal interest, both from a fundamental and industrial perspective.[1] Inspired by previous ultra-high vacuum studies performed on model single-atom Pd/Fe3O4(001) catalysts activating the low-temperature methanol to formaldehyde oxidation,[2] a series of model Rh/Fe3O4(001) catalysts were examined for the low-temperature ethanol to acetaldehyde oxidation. Distinct Rh active sites, including Rh adatoms, substitutional in-surface Rh, and Rh clusters, were prepared using different preparation conditions and amounts of Rh.[3] The Rh catalyst structures and activities were characterized by combining thermal desorption and photoelectron spectroscopies, and it was found that all model catalysts significantly reduce the temperature of the acetaldehyde production when compared to the bare Fe3O4(001) surface. There are, however, significant differences in the selectivities, not just between Rh single-atoms and clusters but also among the different single-atom species. We will highlight how the local environment characteristic of Rh single-atom catalysts influences their performance and establish their dynamic response to coordination of carbon monoxide while Rh clusters suffer from poisoning. As our surface science approach allows us to control the coordination sphere of Rh centers with ultimate precision, we can establish

how similar concepts can be applied to homogeneous and heterogeneous single-atom catalysis.

[1] J. Gong, C. B. Mullins, JACS 2008, 130, 16458-16459.
[2] M. D. Marcinkowski, et al., ACS Catalysis 2019, 9, 10977-10982.
[3] a) M. A. Sharp, et al., JPCC 2022, 126, 14448-14459; b) Z. Jakub, et al., Nanoscale 2020, 12, 5866-5875.

Friday, August 29, 11:00 AM: **Atom Probe Tomography Analysis of Sigma 3 Grain Boundaries in Sensitized 316 Stainless Steel Cladding**

Francelia Sanchez, Semanti Mukhopadhyay, Dallin Barton, Jaqueline Royer, Kayla Yano, Jenna A. Bilbrey, Arun Devaraj
Pacific Northwest National Laboratory

316 Stainless steel (316 SS) is used as the cladding for tritium producing burnable absorber rods because of its high temperature strength and excellent corrosion resistance. However, the material is susceptible to sensitization and radiation induced segregation to grain boundaries. Understanding grain boundary segregation is crucial for predicting material behavior and optimizing the performance of 316 SS under extreme environments. These localized compositional changes can negatively impact the material's properties, potentially causing intergranular corrosion cracking and premature failure. In this study, the elemental distribution across a $\Sigma3$ grain boundary in sensitized 316 SS cladding was investigated using atom probe tomography (APT), a powerful technique that provides 3D elemental mapping with near-atomic resolution. APT samples were prepared using a dual beam xenon plasma focused ion beam scanning electron microscopy equipped with an electron backscatter diffraction detector, used for analysis of grain boundary character. The results provide detailed insights into the elemental distribution and chemical quantification of alloying elements across special grain boundaries.

Friday, August 29, 11:20 AM: **Age-linked variations in dental enamel nanostructure and fluid permeability revealed by atom probe tomography**

Jack Grimm, Katherine Tang, Cameron Renteria,
University of Washington
Arun Devaraj,
Pacific Northwest National Laboratory
Dwayne Arola,
University of Washington

Human dental enamel is a critical component of a healthy lifestyle, both in terms of its ability to resist fracture over decades of use as well as to present an aesthetically pleasing smile. The remarkable damage tolerance is a product of a complex hierarchical microstructure with features ranging from decussation bands (~50 µm) to rods (~5 µm) to hydroxyapatite nanocrystals (~50 nm). The nanocrystals are of particular interest for several reasons including: (i) compositional gradients within single nanocrystals have been proposed to improve mechanical properties and resistance to dissolution, (ii) normal and pathological de- and re-mineralization begin at the nanocrystal scale, and (iii) organic precipitates between nanocrystals may be connected to both mechanical properties and enamel aesthetics. How these nanoscale features vary as a function of aging is an important question underpinning design of treatments and products for an aging population.

Nanocrystals present a challenge for many characterization tools, but atom probe tomography has the spatial (~1 nm) and compositional (up to ~ppm) resolution to illuminate differences between Primary, Young, and Senior enamel nanocrystals. In this presentation, we compare the composition of nanocrystals, the intergranular spaces between them, and organic precipitates from inner enamel samples, revealing an apparent absence of Mg-rich cores previously presumed to be universal in human enamel. Additionally, we exposed the samples to an NaOCl bleaching treatment, finding evidence that the Primary enamel is more responsive than Young or Senior enamels. These insights improve our understanding of how enamel changes with age, and how to optimize treatments.

Friday, August 29, 11:40 AM: **Interlayer engineering improves reverse bias stability in halide perovskite photovoltaics**

Fangyuan Jiang
University of Washington

Reverse bias instability represents a major challenge to both the reliability and large-scale deployment of halide perovskite photovoltaics. Reverse bias arises when one cell in a series-connected module becomes shaded, generating less power than its neighbors. The unshaded cells then impose a reverse voltage on the shaded unit, forcing current to flow in the wrong direction and triggering severe device degradation. In this work, we demonstrate that interlayer engineering can enhance reverse bias stability under two distinct operating conditions. The first case involves mitigating cell failure at high reverse bias by suppressing dark current and raising the reverse breakdown threshold, thereby potentially lowering the number of bypass diodes required at the module level. The second case addresses the situation where a shaded cell must conduct large reverse currents (J_{mpp}, the current density at maximum power point), which enables intrinsically stable cells and eliminate the need for bypass diodes altogether. Here we conducted a systematic investigation of degradation dynamics under reverse bias and reverse current stress, examining the influence of illumination intensity, injected current density, and shading fraction. Our findings highlight notable advances in stabilizing devices against reverse current stress, and reveal distinct degradation pathways under high reverse voltage (with relatively low current) versus high reverse current. Furthermore, we propose additional mitigation strategies aimed at overcoming reverse bias challenges in both scenarios.

Graduate Student Posters

G 1: Atomic Layer Deposition of Barium-Based Oxides for Ultrahigh-k Dielectric Applications

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Barium-containing oxides show promise for energy-efficient logic and memory devices. For example, barium titanate (BTO) is a perovskite-ferroelectric with a low coercive field, and barium-hafnium-titanium oxide (BHTO) is an ultrahigh-k dielectric with a high breakdown voltage. Integration of these materials into manufacturing requires scalable, conformal synthesis, with back-end-of-line compatible processes. Atomic layer deposition (ALD) achieves conformal low temperature deposition via self-limiting surface reactions with reactive precursors, but few processes have been reported for barium films. Binary BaO ALD process development has been limited due to challenges associated with barium precursors, particularly their low volatility, which hinders uniform deposition at low temperatures. Furthermore, BaO needs to be deposited in a strict oxygen-controlled environment because of the hygroscopic nature of BaOx, which can easily convert to Ba(OH) or BaCO3 in the presence of oxygen or moisture. This behavior complicates film characterization, as phase identification using X-ray diffraction (XRD) or chemical analysis via X-ray photoelectron spectroscopy (XPS) may detect hydroxide or carbonate species instead of pure BaO, leading to inaccurate composition and electrical measurements. Here, we report progress towards a novel BaO ALD process using an imidazolate-based barium precursor. The deposition characteristics, including ALD temperature window, growth per cycle, and film structure, are investigated at growth temperatures of 150-300 °C. Parameters such as thickness, density, roughness, phase composition, and dielectric constants are examined to assess the feasibility of this precursor for ALD of BaO and its potential contribution towards ternary and quaternary barium-based oxides."

G 2. The Restructuring of Cobalt Telluride Electrocatalysts in the Oxygen Evolution Reaction

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Hydrogen represents one of the most attractive options for energy storage from renewables; it is the simplest and most abundant element on earth and has the highest energy density of any fuel. Driven by the goal of a zero-emission energy infrastructure by 2050, a green hydrogen economy is critical to enable a 100% renewable society. A promising pathway towards sustainable hydrogen production is water-based electrolysis, but a critical barrier for efficient water splitting is the high overpotential of the sluggish oxygen evolution reaction (OER). Among non-noble metals, transition metal chalcogenides have emerged as excellent options due to their superior electrocatalytic performances and electrical conductivity. It is known that transition metal chalcogenides experience restructuring in corrosive and oxidative OER, but it is unknown what triggers such restructuring and whether the final product is metastable. In this study, we used cobalt telluride (CoTe) as a model system and combined in-situ X-ray absorption spectroscopy with ex-situ characterizations to understand restructuring mechanisms. Results suggest that restructuring of Co-Te bonds into Co-O bonds immediately starts when CoTe is immersed in KOH solution, suggesting true active sites of cobalt oxides or oxyhydroxides. The applied voltage can further promote the restructuring, but the restructuring is largely done before OER. Additionally, results suggest that restructuring starts from leaching of Te from the lattice, forming vacancies which are filled with O atoms from the electrolyte. It was also observed that leached Te in the electrolyte could redeposit onto the CoTe, forming TeOx which could influence the overall activity.

G 3. Toward Atomic Layer Deposition of Nitride Compounds Via Integration of Plasma-Assisted Atomic Layer Annealing

Peter Micah, Steven M. Hues, and Elton Graugnard
Boise State University

Plasma-based atomic layer annealing (ALA) uses cyclic low-energy bombardment to achieve improved density, purity, and crystallinity in atomic layer deposited (ALD) films. This approach facilitates low-temperature annealing as an alternative to conventional high-temperature annealing processes, improving electronic properties with a lower overall thermal budget. This study explores the integration of ALA into thermal ALD processes to achieve precise control over the film phase, morphology, and reaction stoichiometry in nitride thin films. To integrate ALA with ALD, a remote plasma source was integrated with a custom ALD system capable of low and high vacuum operation. Previous ALA studies demonstrated that precursor selection plays a crucial role in optimizing successful deposition, with tris(dimethylamino)aluminum ligands in TDMAA (-NMe2) exhibiting superior carbon removal efficiency compared to trimethylaluminum (TMA), thereby enhancing self-limiting reactions and improving film quality. By leveraging organometallic precursors with remote plasma-assisted ALD and ALA, we explore deposition of binary (AlN, GaN & HfN) and ternary (AlScN) nitride dielectric films. Our ALA/ALD methodology includes nano-lamina stack film design and mono-layered laminated super-cycle deposition processing for phase-engineered dielectrics. We will report ALA-ALD process conditions and resulting film properties, including phase, composition, dielectric constant (κ), leakage current, and breakdown voltage using capacitor test devices. Promising films will be used in fabricating energy-efficient logic and memory devices.

G 4. Integrated UHV Chamber for Single-Crystal Electrode Preparation and Air-Free Transfer to Electrochemistry

Collin Smith and Gary Harlow
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We present an ultra-high vacuum system that integrates preparation, characterization, and clean transfer of single-crystal metal electrodes for interfacial electrochemistry. Cycles of Ar+ sputtering (1–2 keV) and e-beam annealing up to 2000 C. Surface quality is verified with a LEED optic covering 35–500 eV. A fast-entry load-lock accepts flag-style sample plates. The system can be expanded to include e-beam evaporation for deposition to metal surfaces or oxide substrates. The system is composed of two chambers separated by a gate valve

where the preparation is performed in the 'clean' side, held at ~1e-9 torr, then transferred across to the analysis chamber where an electrochemical cell is attached by a KF flange behind a pneumatic gate valve. After venting with argon the prepared electrode can be lowered into the cell and connected to a potentiostat for electrochemical experiments. The chamber is equipped with UV bakeout lamps to remove water from the interior after exposure to electrolyte which helps maintain the load-lock pressure to ~5e-7 torr. The integrated workflow delivers atomically clean, well-ordered electrodes to the electrolyte, enabling systematic investigations of electrochemical kinetics and double-layer structure."

G 5. Acetonitrile as a Cosolvent for high-voltage Aqueous Sodium-ion Batteries

Mason Lyons and Zhenxing Feng
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Aqueous electrolyte sodium-ion batteries using iron-based cathode materials have the potential to alleviate the flammability and cost concerns for state-of-the-art lithium-ion batteries with organic electrolyte. To further improve upon the voltage and high-rate limitations of super-concentrated aqueous electrolytes such as 17 mol kg^-1 NaClO4, organic cosolvents are added. Acetonitrile (AN) is a good candidate due to its miscibility with water, high dipole moment, and median dielectric constant which preserves salt solubility and extends the voltage stability. To understand the role of AN content, mixtures with varied ratios of H2O-AN saturated with NaClO4 undergo electrochemical stability window testing combined with post-mortem electrolyte and electrode analysis to understand reactivity and degradation mechanisms which occur at the solid-liquid interface. Then, the impact on rate capability and coulombic efficiency of an iron-based Prussian Blue battery cathode is evaluated to determine its feasibility for accommodating high-voltage (> 1 V vs AgCl, saturated KCl) redox.

G 6. Electrochemical Performance and Structural Characterization of Na4FexV2-x(PO4)3 Cathode Material for Sodium-Ion Batteries

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Sodium-ion batteries represent a promising alternative to lithium-ion batteries for large-scale energy storage applications due to sodium's high abundance and enhanced safety

when combined with aqueous electrolytes. My research investigates rhombohedral Na4FexV2-x(PO4)3 (x = 1, 0.75, and 0.5) as a polyanionic cathode material for sodium-ion batteries. Electrochemical testing in organic electrolyte solution (ethylene carbonate: diethyl carbonate, 1:1 v/v) revealed specific capacities of 86 and 68 mAh g-1 for x=0.75 and 0.5, respectively. The x=0.75 composition demonstrated a capacity retention of 91.07% after 600 cycles with a coulombic efficiency of 99.18%. It is hypothesized that this cathode material's two distinct redox voltage ranges could be related to Fe3+/Fe2+ at 2.3-2.7 V vs Na+/Na, and V4+/V3+ at 3.3-3.6 V vs Na+/Na, for a multi-electron transfer mechanism. To approve this hypothesis and understand the storage mechanism, comprehensive structural and chemical characterization was performed using ex-situ X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and combined ex-situ/in-situ X-ray absorption spectroscopy (XAS). In-situ XAS characterization confirmed the oxidation/reduction of Fe and V at their respective voltage plateaus during electrochemical cycling. XRD analysis verified the rhombohedral crystal structure, while XPS provided detailed surface composition information. These results demonstrate the potential of Na4FexV2-x(PO4)3 as a viable cathode material for sustainable energy storage applications.

G 7. Atomic Layer Deposition of Ta_2O_5 on Composite Ni-rich Cathode Electrodes for High-Voltage Lithium-Ion Battery Cycling

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Enhancing the interfacial stability of high-energy lithium-ion battery cathodes is critical for achieving long cycle life under wide electrochemical windows. In this study, we employ atomic layer deposition (ALD) to deposit a conformal Ta_2O_5 thin film directly onto the entire composite Ni-rich cathode electrode, rather than on cathode powders as conventionally practiced. This strategy ensures uniform protection not only of the active materials, but also of conductive carbon and polymeric binders, thereby preserving the electronic conductivity network and structural integrity of electrodes throughout extended cycling. Ta_2O_5, known for its excellent chemical and electrochemical stability, serves as a robust interfacial barrier that mitigates parasitic side reactions and suppresses impedance growth. Electrochemical impedance spectroscopy and surface analyses confirm the effectiveness of the coating in stabilizing the electrode–electrolyte interface. As a result, the capacity retention of Ta_2O_5-coated electrodes was improved by ~30% after 200 cycles at 4.6 V vs. Li^+/Li. This work highlights the advantage of whole-electrode coating in enabling durable, high-voltage lithium-ion battery operation.

G 8. Tuning Surface Reactivity through Al-Doped Supports for CO Activation at the Ru/MgO Interface

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CO activation is an important step in many chemical reactions, including Fischer–Tropsch synthesis (FTS), which transforms synthesis gas (CO and H_2) into long-chain hydrocarbons. While CO activation on Ru is well studied, how support modifications through doping affect the electronic structure and chemical activity remains less understood. MgO is a common catalyst support due to its stability and acidic–basic properties, which can be further tuned through doping. In particular, doping MgO with Al is expected to introduce Lewis acidity and promote oxygen vacancy formation, potentially enhancing catalytic activity at metal–oxide interfaces. In this study, density functional theory (DFT) calculations were used to investigate how doping MgO(100) with Al affects the reactivity of supported Ru catalysts toward CO activation. A model of Ru nanorods supported on MgO is employed, with CO as a probe molecule. We systematically studied the effect of Al doping on the adsorption, activation, and dissociation of CO, as well as subsequent C–H bond formation at the Ru(111)/MgO interface. The results indicate that Al doping does not alter the preferred adsorption site of CO on Ru but increases electron density at Ru active sites, favoring electron transfer to CO and enhancing its stability. Al also facilitates oxygen vacancy formation at the Ru/MgO interface, aiding both CO dissociation and C–H bond formation. These electronic modifications lead to a measurable elongation and weakening of the C–O bond, consistent with enhanced CO activation on Al-doped Ru/MgO catalysts.

G 9. Understanding fundamental properties of Ni—based HEA as a catalyst for CO2RR

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With the continued rise in global CO2 emissions, developing new catalysts for energy-efficient and effective CO2 reduction (CO2RR) is imperative. High Entropy Alloys (HEAs) have been studied as a potential catalytic material with promising applications in electrochemical reactions like CO2RR, oxygen evolution reaction, and nitrogen reduction,

but less is known about the potential of HEAs for thermo-catalytic applications. A theoretical understanding of electronic and structural properties can guide the tuning of the HEA for optimal results. In this study, we used Density Functional Theory to investigate the adsorption behavior of key intermediates involved in CO2RR on an AlCoCrFeNiMnTi HEA. Catalytic descriptors such as vibrational frequencies, adsorption energies, and Bader charge analysis were evaluated to determine how complex compositions of reactive sites affect interaction. The adsorption behavior of the HEA was compared with that of pure metals and bimetallic alloys to evaluate their relative performance and cocktail effects due to the compositional complexity of the surface. Through the DFT calculations, we establish charge transfer trends, adsorption site preferences, and surface restructuring following adsorption. Results illustrate improvement in the adsorption energy compared to pure Ni and other transition metals within the alloy component. These findings provide fundamental insights into the alloy's behavior and offer a foundation for rational design and modification of HEAs for CO2RR and other thermo-catalytic applications.

G 10. Degradation Mechanisms of Iron-Based Prussian Blue Cathodes in Aqueous Sodium-Ion Batteries

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Aqueous batteries have attracted significant attention due to their inherent safety, low cost, and environmental friendliness compared to organic electrolyte-based systems. Despite their promising potential, the commercialization of aqueous batteries—particularly in standardized cylindrical or prismatic cell formats—remains challenging due to issues such as electrode stability, electrolyte decomposition, and material degradation. This study focuses on the performance and degradation mechanisms of Prussian blue analogue (PBA) as a cathode material coated on a titanium (Ti) current collector in an aqueous battery system. Prussian blue and its derivatives are considered promising cathode materials due to their open framework structure, high theoretical capacity, and tunable redox properties. Herein, we systematically investigate the electrochemical behavior and degradation mechanisms of PBA-based electrodes on Ti current collector under different voltage windows. Through a combination of ex-situ X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS), we demonstrate that the capacity decay is closely associated with structural evolution in the PBA lattice, including phase transitions, metal-ion dissolution, and irreversible changes in the coordination environment. This work provides fundamental insights into the failure mechanisms of PBA-based aqueous batteries and offers guidance for improving their cycling stability. By

elucidating the relationship between operating voltage, structural evolution, and performance decay, we propose potential strategies—such as lattice doping, protective coatings, or electrolyte additives—to enhance the durability of PBA cathodes in practical applications.

G 11. Understanding the Growth of ZIF-8 Thin Film and Its Gas Sensing via Quartz Crystal Microbalance

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Metal-organic frameworks (MOFs), particularly zeolitic imidazolate frameworks (ZIFs), have emerged as promising materials for gas sensing applications due to their high surface area and tunable porosity. This study presents a systematic chemical bath deposition (CBD) approach for fabricating ZIF-8 films with precisely controlled thicknesses up to 2.5 μm on functionalized surfaces. Film particle evolution and growth mechanisms were investigated using scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and time-of-flight secondary ion mass spectrometry (ToF-SIMS) combined with in-situ growth monitoring. Imidazolate achieved a uniform growth rate of 95 nm per cycle, and imidazolate-surface interfacial coordination was elucidated. By integrating these controllable ZIF-8 films with a quartz crystal microbalance (QCM), we developed a gravimetric gas sensor that demonstrated enhanced CO_2 adsorption capacity with increasing film thickness and achieved a detection limit of 0.5%. This systematic approach to controlling ZIF-8 film thickness enables precise quantification of gas absorption, advancing the development of high-precision gas sensors for environmental monitoring applications.

G 12. Development of Sorbents for Extraction of Strontium from Seawater

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Oceans are a largely underutilized resource. Developing materials and methods to responsibly harvest and utilize the diverse minerals present in seawater could aid our

national security and boost domestic production of critical minerals. One such element of interest in seawater is strontium (Sr) which has seen increased demand in recent years for usage in ferrite magnets as a cheaper and more environmentally friendly alternative to rare-earth containing magnets. The extraction of Sr from seawater has seen some interest in recent years but remains largely unexplored. Sorbents for selective Sr removal have been previously reported for nuclear waste management, but seawater is a completely new matrix and brings unique constraints both technical and economic that need to be considered. In this work, we report the synthesis and characterization of an ion-exchange material that is selective for Sr in the presence of higher concentrations of competing calcium ions. The silicate-based sorbent is synthesized under varying process conditions and its performance is characterized in synthetic seawater to evaluate sorbent selectivity and capacity, which are then used to identify relationship between sorbent composition, crystal structure, and selective uptake of Sr. Current efforts are focused on evaluating the reversibility of Sr uptake by the sorbent, which is critical to its practical use.

G 13. Nickel-Iron Alloys as Efficient, Earth-Abundant Catalysts for Electrochemical Conversion of Nitrate to Ammonium

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Ammonia production via the Haber-Bosch process is responsible for 3% of global greenhouse gas emissions, and runoff from ammonia-based fertilizers are a significant source of nitrate pollution in waterways that cause harmful algae blooms and poses human health risks. The electrochemical nitrate reduction reaction (NO3RR) is a promising approach to mitigating both problems by converting aqueous nitrate into ammonium. First row transition metals have been widely studied as cathodes for NO3RR, but tend to exhibit a tradeoff between selectivity to ammonium (S_NH4) and overall Faradaic efficiency (FE_NO3RR) – ability to reduce nitrate while avoiding the competing hydrogen evolution reaction. Cobalt is a notable exception in that it has high S_NH4 and FE_NO3RR, but it is toxic and expensive. In this study, we investigate whether NiFe alloys can overcome these tradeoffs and approach the performance of Co. We combine electrochemical measurements with density functional theory (DFT) calculations to understand how alloy composition affects activity and selectivity. Experiments show that NiFe alloys consistently achieve higher S_NH4 and FE_NO3RR than either pure Ni or Fe. DFT results suggest that this improvement arises from a multi-site mechanism, where nitrate adsorbs preferentially at Fe-

rich sites and protons at Ni-rich sites, facilitating reaction steps that favor ammonium over undesired byproducts.

G 14. Developing a Platform for Imaging, Dynamically Tuning, and Optically Probing Moiré Interfaces

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Moiré superlattices of 2D semiconductors are promising platforms for quantum information applications due to their periodic potentials enabling the synthesis of scalable, tunable single-photon emitters. The emitter properties depend on the twist angle between the two atomic lattices, however, and standard techniques for moiré synthesis do not enable the in situ twist angle control necessary to turn moiré sites into useful devices for these purposes. In this project, we aim to develop techniques for situ control of moiré twist angles and near-field optical probing of moiré lattices sites. A sharp tungsten tip mounted on a quartz tuning fork is used to image moiré sites using torsional force microscopy operated with open-source control software; this setup together with a rotating platform and an optical fiber mounted onto the tip will enable the in situ control and optical probing of moiré sites. We present current efforts towards imaging moiré superlattices using our setup, and we explore the next steps towards achieving in situ twist angle control.

G 15. Area-Selective Deposition of Tungsten Selenide

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Microelectronic and photovoltaic technologies require scalable and sustainable fabrication techniques for high-performance semiconductors. Tungsten selenide (WSe_2) is a promising candidate for such applications due to its thickness-tunable bandgap. To address this need, we grew thin films of WSe2 using a hybrid atomic layer deposition (ALD) and chemical vapor deposition (CVD) multi-step approach. First, ALD of tungsten oxide (WO3) was achieved on silicon substrates using tungsten carbonyl (W(CO)6) and water as precursors and nitrogen as the purge gas. Next, CVD of WSe2 was achieved using the WO3 thin films and a solid selenium precursor in a tube furnace. Scanning electron microscopy (SEM) and X-ray diffraction spectroscopy (XRD) were used to assess film morphology and chemical structure. Our next steps involve selective deposition from the bottom up via seed material. Density functional theory (DFT) calculations will be implemented to identify the optimal surface chemistry regarding precursor adsorption onto growth and non-growth areas.

Overall, this work utilizes a less toxic tungsten precursor with more environmentally friendly byproducts to achieve WSe2 thin film growth of varying thickness that can be employed in transistors or solar cells.

G 16. Energy-Efficient Synthesis of $Ni_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) Cathode Precursors via Rapid Single-Step Radio Frequency (RF) Heating

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Ni-rich layered oxides such as $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) are widely used as cathode materials in lithium-ion batteries due to their high energy density. However, conventional synthesis methods for NMCs are energy-intensive, time-consuming, involve multiple processing steps, require solvents, and generate significant wastewater. Additionally, converting NMC sulfate hydroxide to oxide phase poses challenges, as residual sulfates at grain boundaries or surfaces can compromise phase purity, resulting in mixed-phase products with reduced capacity, poor cycling stability, and obstructed Li^+ diffusion. In this study, we present a novel Radio Frequency (RF) - powered reactor capable of synthesizing NMC811 precursor rapidly and energy-efficiently in a single, solvent-free step. This process enables direct conversion of NMC811 sulfate hydroxide to a sulfate-free transition metal oxide. RF heating offers high heating rates, localized volumetric heating, while being non-contact, and material selective.

G 17. Energetics of Methanol Adsorption on H- and CO-Precovered Pt (111) Surfaces

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Understanding the adsorption energy of reactants on metal surfaces is fundamental to catalytic and electrocatalysis, including processes such as methanol synthesis, Fischer–Tropsch synthesis, and hydrogen fuel cells. These adsorption energies provide critical links between the catalyst structure to activity and serve as essential benchmarks for validating computational methods, such as density functional theory. Single crystal adsorption calorimetry (SCAC) is the only method capable of detecting the heat of adsorption of molecules on single crystal surfaces [1]. While interactions between reactants and metal surfaces have been extensively studied, the influence of coadsorbed species such as hydrogen and carbon monoxide remains poorly understood. Here we use SCAC to investigate how strongly bound adsorbates, such as H and CO, affect methanol adsorption and binding on Pt (111). We quantify the differential heat of adsorption of methanol on Pt (111) saturated by (1×1) H and ($\sqrt{3} \times \sqrt{3}$) R30° CO adlayers [2]. The initial heat of adsorption decreases from 65 kJ/mol on bare Pt (111) to ~55 kJ/mol on H/Pt (111) and to ~45 kJ/mol on CO/Pt (111). These results demonstrate the significant impact of coadsorbed species on methanol binding and provide important insights into surface interactions relevant to electrodes and catalytic metal nanoparticles.

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G 18. Tuning ferroelectric properties of hBN via shear deformation

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Tuning lattice constants and crystal symmetries via strain from direct mechanical manipulation allows investigation of properties modified through structural changes. This motivates established methods such as uniaxial tension where properties are measured as a crystal is stretched along a single axis. In layered 2D vdW materials, however, interlayer shifts directly affect symmetries and phases suggesting that shearing rather than pure tension may be a more natural experimental tuning knob. Here we develop a new approach for applying shear deformations to 2D materials and conduct proof-of-principle measurements on the sliding ferroelectric, AB-stacked hBN. Sliding ferroelectrics, a class of ferroelectrics restricted to 2D vdW materials, switch polarization via interlayer sliding at a ferroelectric interface. While materials like WTe2 have crystal structures which allow sliding ferroelectricity, the class of sliding ferroelectrics can be expanded through engineering a ferroelectric interface by stacking. Hexagonal BN is a commonly used 2D dielectric whose AA' stacking order can be modified by parallel stacking to engineer a metastable AB or BA interface. We probe ferroelectricity of stacked hBN by incorporating it into graphene-based transistor devices and carrying out resistivity measurements while applying shear deformations. Deformations are applied using a custom calibrated PDMS-based probe. Ferroelectric switching with electrical control was observed in the AB stacked device and not in the corresponding AA' stacked device. Application of lateral deformation to the ferroelectric device showed gradual tuning of the ferroelectric switching and eventually a larger shift, revealing a new ferroelectric domain in the device not previously accessible with electronic control alone.

G 19. Realization and perspectives of all-optical anti-Stokes thermometry with H3 micro-sized diamonds

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The negatively charged nitrogen-vacancy center in diamond (NV-) has attracted a lot of attention due to its unique spectroscopical characteristics. However, while optically detected magnetic resonance (ODMR) and the Debye-Waller factor thermometry (DWFT) of NV- are versatile tools for measuring temperature, under green laser irradiation NV-containing diamonds experience detrimental photothermal heating, lowering the sensitivity of the sensors [1]. Formation of H3 defects decreases the concentration of the NV- defects. Moreover, under green laser excitation H3 defects have anti-Stokes photoluminescence (PL), which is the evidence of ground state phonon absorption and can potentially mitigate heating, depleting the population of phonons [2].

This work focuses on micro-sized diamonds containing NV- and H3 defects, suitable for micro-scale temperature measurements and underlines high potential of anti-Stokes H3 DWF thermometry. We study the presence and the concentration of NV- and H3 by PL spectroscopy and systematically analyze the degree of heating in different diamond grains. The results of ODMR and DWFT suggest a strong correlation between the concentration of NVs and the observed photothermal heating, proving reduced heating in H3-doped diamonds. By developing anti-Stokes H3 DWFT we demonstrate that the H3 defect could potentially be an excellent solution to the detrimental heating problem in diamond sensors in case the concentration of NVs is significantly reduced.

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G 20. Mapping Populations of Active Species in Radio Frequency Nitrogen Plasma with Quantum and Classical Learning

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Radio frequency (RF) plasma sources are critical for the synthesis and processing of materials. Plasma energetics and the relative concentrations of their species can significantly influence the quality and properties of a material sample. Controlling the characteristics of these plasmas is essential for refining material processes and better understanding the influence that various plasma species have on the growth and processing of material samples and devices. Parameters for RF plasma source operation are traditionally optimized through a process of Edisonian trial–and–error. This iterative approach towards process refinement is expensive in terms of both material resources as well as time spent conducting experiments; however, machine learning techniques offer a rapid approach for recognizing complex patterns and generalizing beyond recorded data to forecast novel, unobserved information. Here, we have recorded optical emission spectra of RF nitrogen plasma for over 2000 various combinations of plasma source operating parameters across a pair of different molecular beam epitaxy chambers and plasma source devices. For each spectrum, the complete set of RF nitrogen plasma source operating parameters is associated with the relative populations of the various species observed within the acquired spectrum. Quantum and classical machine learning algorithms are trained on the extracted data, and the model exhibiting superior generalization performance is implemented to forecast the relative population of each species across a broad processing space of possible operating conditions.

G 21. 3D-MICE: 3D-printed Molecularly Imprinted Carbon Electrode

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Pyrolyzed carbon materials (e.g., granular activated carbon) are widely used to remove toxic, per- and polyfluoroalkyl substances (PFAS) from water but have low selectivity over co-occurring contaminants. To address this limitation, molecularly imprinted polymers (MIPs)— polymer networks with cavities that exhibit selective high affinity toward target analytes can be integrated with pyrolyzed carbon to enhance PFAS selectivity. This work developed 3D-printed, pyrolyzed carbon lattices functionalized with perfluorooctane sulfonate (PFOS)-templated MIPs for selective PFAS removal. High-surface-area lattices were fabricated by stereolithography (SLA) 3D printing of photopolymer resin. The printed structures were first oxygen plasma–etched to increase surface roughness and active site density, then vacuum-pyrolyzed at 900 ∘C to convert the polymer into conductive carbon. A second etching step further improved surface wettability. PFOS-specific MIPs were then deposited onto the carbon via cyclic voltammetry using o-phenylenediamine as the functional monomer (with PFOS as the template). Raman spectra of the pyrolyzed substrate showed characteristic D (1322 cm−1) and G (1605 cm−1) bands, with an ID/IG ratio of ≈ 1.22, indicating a high-defect density structure favorable for polymer nucleation and adhesion. Cyclic voltammetry peaks at 0.62, -0.10, -0.31 V vs Ag/AgCl, along with carbon–nitrogen stretching Raman peaks at 1366 cm−1, 1408 cm−1 and 1485 cm−1, confirmed successful electropolymerization and MIP deposition after PFOS template extraction. Scanning electron microscopy revealed uniform MIP coverage of lattice struts, with the imprinted films exhibiting smooth, continuous morphology. These results demonstrate high accessible surface area and homogeneous MIP coating, underscoring the potential of this material for selective PFAS removal.

G 22. ToF-SIMS and EDX Insights into Oxidation-Driven Cr Migration in High-Entropy Oxides

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High-entropy oxides (HEOs) combine exceptional compositional flexibility with structural stability, making them attractive for energy and catalytic applications. We investigate how Sr doping alters B-site cation oxidation states, composition, and structure in epitaxial $La_{1-x}Sr_x(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$ thin films. X-ray spectroscopies reveal that Sr preferentially oxidizes Cr^{3+} to Cr^{6+}, partially oxidizes Co and Ni, and leaves Mn^{4+} and Fe^{3+} largely unchanged. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) and atomic-resolution scanning transmission electron microscopy (STEM) with energy-dispersive X-ray spectroscopy (EDX) deliver complementary depth-resolved and atomically resolved elemental mapping across different length scales. Both techniques identify pronounced Cr segregation—being depleted at the interface and enriched at the surface—and partial amorphization in heavily doped films. These results indicate oxidation-driven migration of smaller, high-valence Cr cations during growth. The combined ToF-SIMS and EDX approach captures structural context and chemical depth profiles, revealing the interplay between charge compensation, local strain, and compositional fluctuations in HEOs, and guides strategies to tune surface composition and electronic structure for robust electrocatalysts.

G 23. Vapor-phase Deposition of Hybrid Bismuth-based Photoresists

Jane Keth, Duncan Reece, and David S. Bergsman
University of Washington

Public demand for faster computation—driven by artificial intelligence and data-intensive applications—has pushed the development of sub-10 nm processors, where increased transistor density enables faster switching and higher computational throughput. Achieving these small feature sizes requires the use of extreme ultraviolet (EUV) lithography, which in turn demands the development of new photoresists compatible with its short wavelengths and high-resolution patterning requirements. Some current methods for developing photoresists materials include infiltrating vapor-phase or incorporating metal-based

nanoparticles into polymer films. However, these methods face challenges such as film distortion, nanoparticle agglomeration, or poor uniformity. One promising alternative technique for creating photoresists involves using a vapor-phase technique called molecular layer deposition (MLD) to develop hybrid inorganic-organic materials. MLD is a process that can selectively deposit on a surface of interest, control the thickness on the Angstrom-level, and finely tune the composition of the film. In this work, we will discuss using Bismuth-based MLD process to grow novel photoresists. We utilize a custom-built high-throughput reactor capable of simultaneously growing films with different organics of interest, characterizing the resulting thin films, and analyzing their as-deposited stability in ambient, chemical, and thermal conditions. This work allows for further optimization in developing photoresists using MLD-based techniques.

G 24. On the Growth of ZIF-8 Within Polymers Through Vapor Phase Infiltration

Seancarlos Gonzalez, Cecilia Osburn, Joelle V. Scott, Yuri Choe, David S. Bergsman, *University of Washington*

Mixed matrix membranes (MMMs) composed of a continuous polymer with embedded metal-organic frameworks (MOFs) show improved gas separation properties and are a promising material towards the implementation of energy-efficient membrane separations. However, issues associated with solution-based synthesis, such as filler aggregation or poor interfacial compatibility, motivate alternative synthesis strategies. One potential option is vapor phase infiltration (VPI), in which a polymer is sequentially exposed to vapor-phase reactants to grow inorganics in-situ within the polymer matrix. Expanding current VPI chemistries to include the infiltration of MOFs could allow for the conversion of existing polymer membranes into MMMs as a drop-in manufacturing step. Here, we show our progress towards MOF infiltration through a two-stage process. First, acrylonitrile butadiene styrene (ABS) is infiltrated with diethyl zinc (DEZ) and water to form zinc oxide, followed by 2-methylimidazole (2-HmIM) which reacts with zinc oxide to form a MOF known as ZIF-8. The presence and crystallinity of ZIF-8 were confirmed through x-ray diffraction (XRD) and precursor infiltration was confirmed using depth-profiled secondary ion mass spectrometry (SIMS). One challenge in characterizing this system is the possibility that crystalline ZIF-8 is restricted to the polymer surface. To resolve this, surface ZIF-8 was etched away with water and then characterized with XRD, SIMS, and scanning electron microscopy (SEM) before and after etching. Results show that ZIF-8 peak intensity from XRD diminishes after etching, but in some cases, remains after successive etching attempts, potentially suggesting limited infiltration of MOF crystallites and incentivizing further work into MMM development through VPI.

G 25. Molecular Lithography on Moiré Heterostructures

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The ability to reproducibly generate high-quality, nanoscale plasmonic cavities using existing methods is restricted by the resolution limits of top-down lithography, lithography-induced defects, interfacial disorder in 2D heterostructures, and fringing electric fields. Molecular lithography can overcome these challenges. In particular, moiré superlattices open an avenue for the pattering of 2D materials and assembly of new nanostructures. Here we explore a molecular lithography approach to assemble plasmonic cavities enabling the manipulation of surface plasmon polaritons (SPPs) with exceptionally low optoelectronic losses.

G 26. Deposition-Dependent Coverage and Performance of Phosphonic Acid Interface Modifiers in Halide Perovskite Optoelectronics

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In this work, we study the effect of various deposition methods for phosphonic acid interface modifiers commonly pursued as self-assembled monolayers in high-performance metal halide perovskite photovoltaics. We compare the deposition of (2-(3,6-diiodo-9H-carbazol-9-yl)ethyl)phosphonic acid onto indium tin oxide (ITO) bottom contacts by varying (1) the method of deposition, specifically spin coating or prolonged dip coating, (2) ITO surface treatment via acid etching, and (3) use in combination with a second modifier, 1,6-hexylenediphosphonic acid. We demonstrate that varying these modification protocols influences carrier lifetimes and quasi-Fermi level splitting of perovskite films deposited onto the phosphonic-acid-modified ITO. Ultraviolet photoelectron spectroscopy shows an increase in effective work function after phosphonic acid modification. We use X-ray photoelectron spectroscopy to probe differences in phosphonic acid coverage on the metal oxide contact and show that perovskite samples grown on ITO with the highest phosphonic acid coverage exhibit the longest carrier lifetimes. Finally, we establish that device performance follows these same trends. These results indicate that the reactivity, heterogeneity, and composition of the bottom contact help to control recombination rates and therefore device performance. ITO etching, prolonged deposition times for phosphonic acids via dip coating, and the use of a secondary, more hydrophilic bis-phosphonic acid, all contribute to improvements in surface coverage, carrier lifetime, and device efficiency. These improvements each have a positive impact, and we achieve the best results when all three strategies are implemented.

G 27.   Functionalization of Black Phosphorus with Metal Complexes for Electrochemistry

Lauren Peck, Andrei Draguicevic and Alexandra Velian
University of Washington

Black Phosphorus (bP) is a two-dimensional van der Waals material that has the potential to serve as a support for catalytic active sites due to its similarity to molecular phosphines. By leveraging this similarity, atomically precise complex coordination sites can be created on a two-dimensional support using molecular chemistry techniques.1 Solution exfoliated bP nanosheets are functionalized with molecular Re complexes through various attachment chemistries to demonstrate the versatility of synthesizing well-defined complex coordination sites on the surface. The functionalized nanosheets, Re(bpy)(CO)3Cl-bP, Re(CO)3-bP, and Re(phd)(CO)3Cl-bP are characterized through infrared and X-ray photoelectron spectroscopy along with scanning transmission electron microscopy to

confirm that there is a high density of single site organometallic Re(I) centers that are bound to the bP surface lattice. The Re complexes that decorate the surface are similar to Lehn-type molecular complexes that are used for electrocatalytic carbon dioxide reduction (CO2RR).2 Electrochemistry techniques are used to analyze the activity of the Re functionalized nanosheets showing a peak due to a Re reduction event. There is potential for these materials to be active for electrocatalytic applications with Re(phd)(CO)3Cl-bP showing preliminary activity with an onset potential at -1.81V vs Fc/Fc+ to drive CO2RR.

G 28. Wavelength Dependent Photoluminescence Mapping of Phenethylammonium Degradation Under Thermal Stress in Perovskite Solar Cells

Julisa Juarez, Lamtuir Samosir and Alan Zhan
University of Washington

Perovskite solar cells combine exceptional power conversion efficiency with low-cost fabrication, but thermal instability at device interfaces threatens their long-term performance. While 2D PEA-based passivation layers are often introduced to suppress interfacial recombination and enhance stability, their benefits can be offset by degradation pathways activated under stress. Two-dimensional (2D) phenethylammonium (PEA)-based passivation layers are known to undergo deprotonation and cation interdiffusion at elevated temperatures. PEA^+ deprotonates to amines that react with FA^+ in the perovskite disrupting structural integrity and charge transport at the interface. In this work, we employ wavelength-dependent photoluminescence (PL) and time-resolved PL (TRPL) to study the migration of surface-applied PEA into the perovskite bulk during controlled thermal aging. By quantifying changes in surface- and bulk-sensitive PL intensities and lifetimes, we resolve distinct degradation pathways linked to cation loss and redistribution. These findings establish multiwavelength PL as a non-destructive diagnostic for mapping interfacial degradation, enabling rapid feedback for the development of thermally stable, high-performance perovskite solar cells.

G 29. Creating Complex Coordination Environments on the Surface of Black Phosphorus

Andrei Draguicevic, Guodong Ren, Juan Carlos Idrobo and Alexandra Velian
University of Washington

Black phosphorus (bP), a layered 2-dimensional allotrope of phosphorus, exhibits a tunable layer-dependent bandgap and has emerged as a next generation Van der Waals material.

Surface functionalization of bP serves as an important step in modifying the surface reactivity and implanting desired functionalities. Synthetic methods for the precise functionalization of bP are scarce and characterization of the resulting materials often lacks a detailed understanding of the coordination environment at the material surface. The Velian lab realizes organometallic chemistry on the surface by utilizing bP as a material analog to molecular phosphines. In this work, bP is modified with molecular organometallic fragments to obtain distinct, discrete and chemically accessible metallic sites. Infrared active carbonyl ligands on the organometallic sites provide insights on the coordination environment of the surface using diffuse reflectance infrared spectroscopy (DRIFTS). Sequential functionalization of bP with precursors containing orthogonal infrared spectroscopic tags allows for the analysis of differing coordination environments on the surface. X-ray photoelectron spectroscopy (XPS) and scanning transmission electron microscopy (STEM) are used to confirm the metal identities on the surface. The synthesis of bP materials with discrete metal sites that are both directly bound and tethered to the surface may provide an avenue for the synthesis of well-defined bimetallic active sites with differing metal identities on the surface of bP.

G 30. Designer Catalyst Surfaces on Black Phosphorus

Hailey Akins, Andrei Draguicevic, Michael Riehs, and Alexandra Velian
University of Washington

Black phosphorus (bP) is a 2-dimensional, crystalline allotrope of phosphorus consisting of corrugated sheets of tri-coordinate atoms. It exhibits remarkable properties such as a layer dependent band gap (0.35 eV in bulk to 2.2 eV in monolayer) and a high carrier mobility (1000 cm2V-1s-1) that make it desirable for thermoelectric devices and field-effect transistors.1 Furthermore, the basal plane is decorated with a network of lone pairs that impart analogous reactivity to molecular phosphines. Our group has previously demonstrated that this can be exploited to functionalize the surface with atomic precision.2–4 In this work, we present preliminary data on the activity, stability, and structure of a novel bP/Rh hybrid material that is active for cyclohexene hydrogenation. This will allow us to develop strategies to electronically and sterically tune the microenvironment of the active site by leveraging the large quantity of literature regarding phosphine chemistry. In principle, this could provide a heterogeneous analog to 'designer' phosphine ligands and expand the otherwise limited strategies for chemically tuning heterogeneous catalysts.

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Undergraduate Student Posters

UG 1. Tuning Properties of Polyethersulfone Membranes via Vapor Phase Infiltration

Alyssa Hicks, Yuri Choe, David S. Bergsman,
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Industrial chemical separation processes, such as distillation, drying, and evaporation, account for 10-15% of U.S. energy consumption. Membranes, which act as selective barriers to separate compounds, are substantially more energy-efficient than traditional heat-driven separation methods. Inorganic membranes are inherently suitable for many separation processes due to their chemical and thermal stability; however, they are mechanically fragile and costly to produce. In contrast, commercial polymeric membranes offer a more economical alternative but are susceptible to degradation in harsh organic solvents and high-temperature environments. Vapor phase infiltration (VPI), a gas-phase synthesis technique involving sorption, diffusion, and entrapment of vapor-phase reactants into polymers, has emerged as a promising strategy to enhance membrane performance. The incorporation of inorganic oxides into polymeric membranes through VPI has been shown to yield hybrid membranes with improved chemical and thermal stability at low cost. However, the mechanical properties of these hybrid membranes, which are crucial for maximizing their lifetime and durability, are generally less well understood. In this study, polyethersulfone membranes were subjected to trimethylaluminum and water under various VPI process conditions in a custom-built reactor. The extent and depth of inorganic infiltration were analyzed using thermogravimetric analysis and time-of-flight secondary ion mass spectrometry. Mechanical performance was evaluated through dynamic mechanical analysis and burst pressure testing, while enhancement in chemical stability was assessed by measuring degradation after solvent exposure. These results provide insight into the relationship between infiltration structure, membrane stability, and mechanical properties, which may inform improved membrane design and support more sustainable industrial chemical operations.

UG 2. Recovering Cobalt and Nickel Ions from Critical Solutions in the Presence of EDTA via Electrodialysis

Jonah Buck and Samuel Perkins
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Cobalt and nickel are toxic heavy metal ions often found in waste solutions from battery recycling and energy product manufacturing facilities. Both are classified as critical materials by the United States and other governments due to their importance in energy technology and national security. However, their similar atomic radii and identical charge makes traditional separation techniques largely ineffective. Prior research has been performed into the selective conjugation of ethylenediaminetetraacetic acid (EDTA) with nickel over cobalt to form an anion to facilitate better electrochemical separation. This study investigates electrodialytic separation in the presence of EDTA as a solution for recovering the critical materials from industrial wastewater solutions. Using a BED 1-2 electrodialysis bench from PCCell GmbH (Germany), we use various ion exchange membrane configurations to draw the Ni(EDTA) anions out of an acidic solution consisting of equal parts cobalt and nickel and an Ni:EDTA ratio of 85:100 by mass. The supporting ions are sulfates (sulfuric acid, metallic sulfate hydrates). Preliminary analysis using inductively coupled plasma optical emission spectroscopy (ICP-OES) shows that over 70% of nickel can be effectively extracted from a solution containing cobalt with this method, with minimal cobalt co-transport. Ongoing experimentation aims to optimize various experimental variables such as membrane selection and current density to increase separation efficiency. EDTA-assisted electrodialysis is a promising strategy for critical metal recovery from industrial wastewater in a potentially scalable and environmentally conscious manner. Recovered materials could then be reused in their respective processes.

UG 3. Quantifying Coverage Effects of HDO-Relevant Aromatics on Fe(110) Using Mean-Field Models

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Washington State University and Pacific Northwest National Laboratory

The growing demand for renewable energy has spurred interest in catalytic conversion of bio-oils into usable biofuels. These biofuels can be upgraded via hydrodeoxygenation (HDO), a process that cleaves C–O bonds. First-principles modeling provides a framework to

describe this process and enables direct correlation with experimental data on bimetallic catalysts, which often pair earth-abundant and precious metals to exploit synergistic effects. Under realistic conditions, however, lateral adsorbate interactions significantly influence reaction pathways and must be accurately captured for predictive modeling. Our previous work demonstrated that the coverage-dependent adsorption of benzene [1] and phenol [2] on Pt(111) can be described using a mean-field model where adsorption energy is an analytical function of coverage, aligning well with calorimetric data [1,2]. This model has been extended to other aromatics on noble metals like Ru [3], but noble metals are not economically viable at scale. This study investigates the coverage-dependent adsorption energies of aromatics (benzene, phenol, anisole, benzoic acid, catechol, guaiacol, toluene, and salicylic acid) on Fe(110), an earth-abundant surface, and evaluates whether their behavior can similarly be captured by a mean-field approach. We hypothesize that establishing a database of these adsorption energies will enable the predictive modeling of functional group behavior across aromatic systems, as variations arise primarily from substitutions on the benzene ring.

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UG 4. Effects of Layer Thickness and Composition Ratios on Layered Ultrathin Metal-Selenium Binary Films

Henry Hutley, David C. Johnson, and Celsey Price
University of Oregon

In thin-film metal-chalcogenide materials synthesis, it is typical that reactions occur differently depending on metals used, the ratio of thickness of the layers deposited, and the targeted thickness of the repeated layering sequence. While computational methods can be utilized to predict how a binary system will react on deposition and post-annealing, it becomes vital to know which synthetic approach one should take to form a desired material. The behavior of metals reacting with selenium as deposited can influence the synthetic outcome of a film. Ultrathin layered metal-selenium Binary systems have been investigated thoroughly by members of the materials chemistry research department at UO. Layer thickness becomes important in these systems as the formation of crystalline structures is

known to be highly diffusion-limited, suggesting that with thinner layers, nucleation is more abundant. Here, we seek to answer the question of what causes metal atoms to diffuse through layers of selenium to the extent that is observed. To approach this, we draw similarities and differences in the way different metals (Pb, Fe, Cr, Nb) interact in selenium environments with varied layer thicknesses and composition ratios. To follow the reaction pathways, we use diffraction patterns (XRD) to indicate any present crystalline or layered structures, as well as X-ray fluorescence (XRF) to determine composition ratios, combined with low-temperature annealing steps. We hypothesize that this difference depends on preferred oxidation states of metal atoms, and how they interact with selenium to quickly lower the free energy of a system with minimal energy input.

UG 5. High Performance Electrolyte for Rechargeable Zinc Batteries with Co-Solvents

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Seattle Pacific University
Ajay Karakoti, Dan Thien Nguyen, and Vijayakumar Murugesan
Pacific Northwest National Laboratory

Batteries are expected to play a critical role in grid scale stability and resilience; however, existing battery chemistries fall short of meeting the DOE goals for the stability and resilience of the nation's power grid. Zinc-based batteries, an emerging class of rechargeable zinc batteries, offer a promising alternative due to their low cost, long duration, and potential for large-scale, sustainable energy storage. Despite their advantages, zinc batteries are hindered by issues such as zinc dendrite formation, hydrogen evolution reactions (HER), and inadequate cathode wetting. Addressing these challenges involves optimizing the co-solvent ratios in the electrolyte. In this study, a high-performance electrolyte was developed by varying the volume ratios of water and sulfone. The optimized electrolyte exhibited excellent cycling performance of the zinc metal anode at high current densities and high areal capacities, eliminating zinc dendrites. Surface characterization techniques revealed improved plating/stripping morphologies and stable electrode interphase compositions. This advanced electrolyte formulation paves the way for highly efficient zinc-based batteries, offering a cost-effective, sustainable grid-storage solution and advancing DOE efforts towards clean, affordable, secure, and resilient energy.

UG 6. The Return of The Molecular Volcano: Polar Distortion

Amal Berhan and Loni Kringle,
Pacific Northwest National Laboratory

Water, the universal requirement for life, has many strange properties that are not clearly understood. We are concerned with the anomalies of deeply supercooled liquid water (30-160 K) in ultra-high vacuum (≤10-10 torr). At these conditions, the metastable and disordered configuration of solid water, amorphous solid water (ASW) is formed. Previous experiments with temperature-programmed desorption demonstrate that the crystallization of ASW precedes the desorption of an underlayer of inert and nonpolar adsorbates; this yields in the abrupt desorption of trapped gases coined the molecular volcano. We couple temperature-programmed desorption and reflection absorption infrared spectroscopy to characterize how polar adsorbates alter the crystallization dynamics of ASW at the vacuum interface. Interestingly, we find that the molecular volcano does not happen with polar adsorbates. Instead, a seemingly strong interaction occurs between the polar adsorbates and ASW. Further quantitative investigation must be conducted to fully understand the kinetics of this interaction.

UG 7. Spectroscopy Atlas of Proteinogenic Amino Acids

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Oak Ridge National Lab

In the field of biology, proteins are widely studied. This makes the building blocks of proteins, amino acids highly relevant for research, often as biological markers to indicate health or disease. The metabolism of amino acids has been shown to control tumor growth and the starvation of certain amino acids has shown to aid cancer immunotherapy, known as 'starvation therapy'. Considering the importance of amino acids in these studies, it is pertinent to fully characterize the 20 so-called common proteinogenic amino acids, the building blocks of all proteins relevant for life. Such characterization can aid research by speeding up the process of identifying amino acids. Additionally, with the recent advent of monochromated electron energy loss spectroscopy (EELS) in the electron microscope, there exists an exciting opportunity to closely study amino acids in a new way. Here, a comprehensive list of relevant characterization data (FTIR, Raman, Neutron Scattering, monochromated EELS, XPS, and their vibrational peak assignments) is provided. The hope

is that by having relevant data in one location, allowing easy comparison between the inelastic cross sections of different characterization data, this paper can aid in the research of thousands of scientists.

UG 8. Toward erosion-corrosion modeling of surface wear from particles at high temperatures

Donagh Palmer, Anders Johnson, Tim Kowalczyk and Nipun Goel
Western Washington University

The use of solid particles as the heat transfer medium in concentrated solar power (CSP) plants is a technology under active development. Understanding the abrasion and corrosion of the particles at high temperatures is essential for chemically and mechanically optimizing the design of solid-partcle heat transfer systems for CSP.[1] In recent previous work, we implemented a model to predict erosive wear using the Discrete Element Method.[2] In this work, we assess the performance of the erosive wear model at higher temperatures and seek to introduce corrosive wear directly into the model to improve its accuracy. We perform reactive forcefield (ReaxFF) molecular dynamics sampling on model iron and iron oxide surfaces to monitor redox reactions on the solid particle surfaces. The simulations will be used to gather surface corrosion kinetics data that can be introduced into the abrasive erosion model.

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High School Student Posters

HS 1. An AI-Powered Mobile Application for chemical safety

RISHI VIJAY
Hanford high school

As the materials R&D community continue to develop new chemicals and advance technological applications, the complexity of household products increases, often introducing hidden risks. This has resulted in over two million chemical poisonings annually in the U.S., with the majority caused by everyday household items. My project, ChemSafe, addresses this challenge by bridging the gap between complex materials data and public safety. The app leverages AI-driven optical character recognition (OCR) to identify ingredients from product labels. Acting as a ""digital chemist,"" it then accesses and interprets underlying Safety Data Sheets (SDSs) and other databases to provide users with instant, easy-to-understand summaries of potential hazards and corresponding emergency protocols. This project showcases a powerful, real-world application of AI in translating complex materials science into practical, life-saving consumer safety information.

HS 2. UiO-66/PANI Nanocomposites Based Chemical Sensors for Enhanced Gas Sensing

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Crescent Valley High School
Tzer-Rurng Su, Haori Yang and Chih-hung Chang
Oregon State University

Metal-organic frameworks (MOFs) are a class of highly porous crystalline materials composed of metal ions connected by organic linkers. Their exceptionally high surface areas along with the functionalities of other materials offer great potential for sensor capability improvement. In this study, we utilized University of Oslo-66 (UiO-66), a zirconium-based MOF known for its chemical stability, as a structural agent to modify amorphous conductive polyaniline (PANI) to form a nanocomposite film. When using the optimal UiO-66-to-PANI ratio, this composite maximizes analyte interaction while maintaining adequate conductivity as a semiconducting material. We synthesized composite materials by polymerizing PANI around preformed UiO-66. Scanning electron microscopy (SEM) was performed to assess

PANI coverage and transmission electron microscopy (TEM) to evaluate UiO-66 distribution. Brunauer-Emmett-Teller (BET) analysis confirmed that the addition of UiO-66 to PANI increased the composite's surface area. We fabricated gas sensors by depositing composite thin films of the UiO-66/PANI onto device platforms using airbrush spray printing. Conductivity measurements showed that lower weight-percent additions of UiO-66 did not compromise PANI's ideal resistance range for chemiresistive sensing. Analysis of sensor performance showed that the addition of UiO-66 to PANI significantly enhanced gas detection of low concentrations ammonia. Additionally, sensor stability and selectivity were evaluated. The sensor was able to detect a wide range of concentrations and achieved a lowest detection limit of 100 ppb. These findings contribute to research on next-generation gas sensors with enhanced sensitivity and practical utility.

General Posters

PS 1. XPS surface chemical analysis for battery materials development

Chris Moffitt and Jonathan Counsell,
Kratos Analytical

The development of materials systems to act as energy conversion and storage systems is a focus in much of the research community, so the need to measure the surface chemical states in these systems continues to grow. This holds true for existing technologies as well as the alternate materials systems being investigated to supplant the current lithium-ion battery LIB systems. Developments in x-ray photoelectron spectroscopy (XPS) systems continue to advance to meet these needs. Results from recent developments in XPS measurement are presented. These include the ability to now profile solid state LIB systems while minimizing the migration of Li ions in the etching process, revealing consistent stoichiometry and eliminating the buildup of Li at interfaces. Advances in sample handling are also discussed, allowing the deconstruction of LIB button cells at different charging cycle intervals, which reveals the chemical changes taking place in the charging process, and the depth distribution of these changes revealed with use of a higher photon energy source in HAXPES (hard x-ray photoelectron spectroscopy) analysis.   Finally, the combinatorial analysis of a Ni-ion battery materials system is discussed, revealing the power of consistent, automated analysis in exploring the chemical trends across composition and material phase variations.

PS 2. Characterization of Batteries Using EIS and Nonlinear EIS

Rebecca Vincent, Yuefan Ji, Rose Y. Lee, and Daniel T. Schwartz
University of Washington

Linear electrochemical impedance spectroscopy (EIS) has long been used to non-destructively characterize batteries and other electrochemical cells in both academia and industry. The Schwartz group has been pioneering the use of 2nd harmonic, nonlinear EIS (2nd-NLEIS) in combination with traditional EIS to improve physical models of charge transfer and diffusion at different interfaces and materials inside a cell.[1,2] This technique can also uniquely characterize charge transfer asymmetry in a cell (for example, differences

between insertion and deinsertion of lithium into an electrode), which is similar to the principal of optical second harmonic generation being used to characterize the centro-symmetry of a single crystal. The Schwartz group is using 2nd-NLEIS to characterize charge transfer mechanisms in lithium metal batteries, as well as health and aging in commercial Li-ion batteries. Our in situ technique and model can finally connect insights from half cells and full cells without requiring a synchrotron; in fact, it requires no new instrumentation for researchers who already use EIS, but rather more attention to how the amplitude of the input current affects the magnitude of the output voltage at 2x the input frequency. Non-destructive study of Li-ion battery state of health is broadly useful to researchers studying cell degradation and to consumers who wish to triage used batteries for second-life applications like stationary storage systems.

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PS 3. Systematic Study on Sodium-based Solid-State Electrolytes to Realize Improved Ionic Conductivity

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Pacific Northwest National Laboratory

Solid state batteries have attracted significant attention in recent years due to their potential to overcome the limitations of conventional rechargeable batteries by enhancing safety and energy density. Among them, all-solid-state sodium-ion batteries (ASSBs) are promising alternatives to lithium counterparts, yet progress is limited by the lack of sodium solid electrolytes with high ionic conductivity, chemical/mechanical stability, and compatibility with high-voltage sodium cathodes and complex material synthesis processes. To address these challenges, halides and oxyhalides have gained attention as promising candidates for sodium solid state electrolytes. In this work, we synthesized oxychloride-based material via mechanical ball milling and carefully optimized annealing, using multimodal characterization to examine their material characteristics and ionic conductivity by minimizing impurities.

PS 4. Solid State Synthesis and Characterization of Hybrid Organic-Inorganic Halides

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Pacific Northwest National Laboratory
Felipe Chavez, Ryan Prieto-Lopez, Joyce Pham
California State University San Bernardino
Kavin Chakravarthy Thangaraj
Washington State University

Understanding the relationships among a material's chemical composition, crystal structure and resultant properties is crucial in many applications, including non-linear optics, quantum materials, and complex magnetism. Controlling the chemical composition of an inorganic solid by introducing an organic component is one means toward designing new materials. The optimization of new hybrid organic-inorganic halides utilizing fundamental chemistry principles (e.g., electronegativity, atomic size, etc.) via solid state synthesis will be discussed. Structural details on the asymmetric units, metal coordination, and choice of organic compositions with their spatial disorders along with in-situ variable-temperature characterization of phase (trans)formations are presented.