37th Annual Symposium of the Pacific Northwest Chapter of AVS, The Science and Technology Society

ABSTRACT BOOK

September 9-11, 2026
Discovery Hall
Pacific Northwest National Lab
Richland, WA

37th Annual Symposium of the Pacific Northwest Chapter of AVS, The Science and Technology Society

Plenary Talk

Thursday 8:00 – 8:30 PM: Surfaces at Scale: AI-Driven Discovery of Catalysts, Sorbents, and the Autonomous Laboratory

Presenter: Vinod Konaganti, Amazon, Worldwide Sustainability

Materials innovation remains a major bottleneck for scalable sustainability technologies, with traditional discovery and deployment timelines often spanning 15-20 years. This keynote presents Amazon Sustainability Science & Innovation's work on autonomous science through AIDE, an AI-driven discovery engine that integrates computational materials design, machine-learned interatomic potentials, AI-assisted synthesis planning, robotic experimentation, and active-learning feedback loops. Candidates are enumerated combinatorially over curated crystal prototypes and a defined metal set, then triaged on formation energy relative to the convex hull by consensus across independent machine-learned potentials, with model disagreement escalated to density functional theory rather than averaged. Survivors are scored on surface adsorption descriptors and, on the shortlist, on reaction barriers; each stage an order of magnitude more costly per candidate, so the experimental budget goes to the few materials worthmaking. The primary case study is catalyst discovery for ultra-low carbon fuels: earth-abundant candidates ranked for hydrodeoxygenation of bio-derived oils on activity and selectivity. We are making the shortlisted candidates both in-house and at academic partners (MIT, JHU, VT, UW), testing, closing the loop back into the models. The same workflow extends to other adsorption-governed materials, illustrated with desiccants and sorbents for cooling and water management, with critical-mineral recovery next. The talk also describes Amazon's S.M.A.R.T. Lab, where robotic synthesis is being commissioned, alongside the physical-AI work that will run it - policies learned from human demonstration and rehearsed in simulation and highlights how autonomous discovery can compress the path from hypothesis to validated candidate.

Invited Talks

Thursday 8:20 – 9:00 AM: Surface Engineering of Gold Nanorods for Enhanced Sensing Performance
Presenter: Ying Bao, Western Washington University

Metal nanocrystals have attracted significant interest due to their unique localized surface plasmon resonance (LSPR) properties and broad applications in sensing, catalysis, and biomedicine. These properties are highly dependent on key physical parameters, including morphology and surface chemistry. The Bao Group aims to enhance the plasmonic performance of metal nanoparticles through controlled nanocrystal synthesis and surface modification. In this talk, Dr. Bao will present recent work on the surface engineering of gold nanorods (AuNRs) for improved mercury sensing. Owing to the high sensitivity of their longitudinal plasmon resonance to changes in particle dimensions, AuNRs serve as promising platforms for mercury detection via amalgamation. However, conventionally synthesized AuNRs stabilized by hexadecyltrimethylammonium bromide (CTAB) often exhibit limited stability and reduced sensitivity due to the dense surfactant layer on the nanorod surface. To address these limitations, we developed PEG-modified AuNRs (PEG@AuNRs), which show enhanced stability in complex environments and enable more effective sensing by promoting reactions at regions of the nanorod surface with the highest plasmonic sensitivity. Additionally, the dynamic range of plasmonic response to mercury concentration can be tuned in this system. If time permits, Dr. Bao will also briefly discuss recent efforts in surface modification of plasmonic nanomaterials for broader functional applications.

Thursday 9:00 – 9:40 AM: Synthetic control of cation distribution and defect formation in high entropy oxides for water oxidation
Presenter: Le Wang, Pacific Northwest National Laboratory

High-entropy oxides offer a powerful platform for water oxidation because multiple cations can create diverse local bonding environments, broaden adsorption-energy landscapes, and improve tolerance to reaction-induced defects. However, in epitaxial high-entropy oxide thin films, the intended random cation distribution can be disrupted by nonequilibrium growth, segregation, and defect formation. In this talk, I will discuss epitaxial La(Cr0.2Mn0.2Fe0.2Co0.2Ni0.2)O3 thin films as a model B-site high-entropy perovskite oxide for the oxygen evolution reaction. Under high oxygen partial pressure growth, the films show high structural quality but develop pronounced Cr segregation, with Cr enrichment near the surface and depletion near the interface, leading to reduced OER activity and stability. By lowering the oxygen partial pressure during pulsed laser deposition, Cr segregation can be suppressed, while a La- and oxygen-deficient perovskite-like phase is stabilized. X-ray spectroscopy, EXAFS, and theoretical calculations reveal selective Co redox and Co/Ni-centered local structural changes consistent with short-range rock-salt-like motifs.

This low-oxygen-pressure phase exhibits enhanced OER activity, improved durability, and strong structural retention, highlighting growth-controlled cation distribution and defect chemistry as key design parameters for robust high-entropy oxide electrocatalysts.

Thursday 10:40 – 11:20 AM: Nanoscale conversion mechanisms in iron oxides control reactivity for electrified steelmaking

Presenter: Paul Kemple, University of Oregon

Raj Shekhar, University of Oregon
Casey Mezerkor, University of Oregon
J. David Bazak, Pacific Northwest National Laboratory
Semanti Mukhopadhyay, Pacific Northwest National Laboratory
Arun Devaraj, Pacific Northwest National Laboratory

Reduction of iron oxides to metal for steelmaking leads to a similar quantity of carbon dioxide emissions to all passenger vehicles. Electrified production of iron can potentially eliminate these emissions and the direct reduction of iron oxide to iron metal can be accomplished at low temperature (<100 C) in concentrated alkaline electrolytes. We set out to understand how the size, composition, and porosity of iron oxide materials influenced their reactivity towards iron metal. Correlated electron microscopy of iron oxides revealed distinct changes in reaction products based on the porosity of the starting material. Rotating-ring-disk electrochemistry revealed the presence of a soluble Fe2+ intermediate which depends on the phase and morphology of the oxide. In-situ magnetic resonance measurements support the presence of long-lived dissolved intermediates and suggest structural differences in reduced hematite. These learnings were used to identify a process to activate scalable iron ores for reduction in low-temperature electrowinning cells, which produced iron at absolute current densities >160 mA cm-2. From these results we propose a few potential pathways and research challenges for electrified iron making for steel manufacturing.

Thursday 1:00 – 1:40 PM: Defect and Interface/Interphase Engineering in Electrode Materials for Rechargeable Batteries

Presenter: Hui (Claire) Xiong, Boise State University

Recent studies have shown enhanced physiochemical properties in metal oxides that containintentional structural defects (e.g., vacancies and interstitials) or with tailored interfaces/interphases for energy storage application. In this talk, recent works in my group including engineering defects in electro ceramic materials through ion irradiation, and electrochemical cycling, as well as studies of solid electrolyte interphases for metal and metal ion batteries will be discussed. Perspectives regarding new pathways to design and engineering defects and interfaces in functional electrode materials will be given.

Thursday 4:00 – 4:40 PM: Ligand-controlled selectivity of single atom catalysts: oxidation of ethanol by Rh/Fe3O4(001)

Presenter: Benjamin Jackson, Pacific Northwest National Laboratory

Daniel Baranowski, Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, Washington 99354, United States
Marcus A Sharp, Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, Washington 99354, United States
Zbynek Novotny, Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, Washington 99354, United States
Liney Arnadottir, Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, Washington 99354, United States
Zdenek Dohnálek , Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, Washington 99354, United States

Supported single-atom catalysts (SACs) offer opportunities to tune catalytic activity and selectivity through the coordination environment of individual metal centers. Here, atomically dispersed Rh on Fe_3O_4(001) is used as a model catalyst to demonstrate ligand-controlled selectivity during ethanol oxidation. Temperature-programmed desorption and X-ray photoelectron spectroscopy show that Rh activates the low-temperature conversion of ethanol to acetaldehyde through a Rh-bound ethoxy intermediate. A fraction of the acetaldehyde subsequently undergoes decarbonylation, producing methane and strongly bound CO. The resulting CO remains coordinated to Rh, transforming the active site from an ethoxy–Rh–ethoxy complex into an ethoxy–Rh–CO complex. This change in coordination suppresses further acetaldehyde decomposition and increases selectivity toward acetaldehyde. Density functional theory calculations map the reaction pathway and explain how CO ligation modifies the geometric and electronic environment of the Rh center, inhibiting the secondary reaction. These results illustrate the dynamic coordination complexes that SACs form under reaction conditions and how selectivity can be regulated by strongly bound reaction products, providing a molecular-level strategy for designing more selective and resource-efficient catalysts.

Friday 8:00 – 8:40 AM: Bringing Acid Catalysis into Electrocatalysis: How Acid Sites Promote Glycerol Oxidation on Pt

Presenter: Kim Juye, Oregon State University

Acid sites are widely used in heterogeneous catalysis, but their role in electrocatalysis remains much less understood. In this work, we investigate the effect of acidic Al sites on the electrocatalytic glycerol oxidation reaction by integrating Pt nanoclusters with a zeolite-templated conductive carbon framework containing acid sites. The optimized PtAlYTC catalyst showed significantly enhanced glycerol oxidation performance under neutral conditions, including an approximately 30-fold higher turnover frequency and 17-fold higher reaction rate than an acid-site-free Pt catalyst. The main products were glyceraldehyde and glyceric acid, while product selectivity changed only modestly,

indicating that acid sites primarily enhance activity rather than alter the reaction pathway. DFT calculations suggest that the acidic Al sites modify the electronic environment of Pt and act as hydrogen acceptors, facilitating dehydrogenation and stabilizing key intermediates. These results highlight a cooperative role between metal and acid sites and demonstrate a strategy for extending concepts of metal–acid catalysis into electrocatalytic systems.

Friday 10:00 – 8:40 AM: Early Career Award Talk:
3D Atomic Strain Mapping of Er:CeO2 Using Multislice Electron Ptychography
Presenter: Elle Schnee , University of Oregon

Joeson Wong, University of Chicago
Cleva Ow-Yang , ThermoFisher Scientific
F. Joseph Heremans, Argonne National Laboratory
Jiefei Zhang, Argonne National Laboratory
Kayla X. Nguyen, University of Oregon

Qubits, quantum network devices, and quantum memory possess spin dependent physical interactions that rely on atomic defects such as dopants. Understanding the impact of dopants on material structure at the atomic scale is crucial for design and manufacturing of quantum devices. Multislice electron ptychography (MEP) is an iterative reconstruction method that solves for the 3D atomic potential of a sample with a single four dimensional scanning transmission electron microscopy (4D-STEM) dataset. In this talk, I will explore the application of MEP to a system of stacked erbium doped cerium oxide nanocrystals—a stable platform for quantum networks. With the atomic potential, we can study bulk and surface properties such as strain, displacement, and atomic density in search of dopant atoms.

General Talks

Thursday 9:40 – 10:00 AM: Navigating Metastability: Predictive and Unconventional Approaches to the Synthesis of Rare Earth Silicon Pnictides

Presenter: Gayatri Viswanathan, Iowa State University

Gordon Miller, Rice University
Kirill Kovnir, Iowa State University

Conventional solid state synthesis often favors thermodynamically stable phases, missing elusive metastable compounds that host diverse crystal chemistry and exotic properties. Metal tetrel pnictides offer a promising space for exploration of candidate quantum compounds with great structural diversity, yet this phase space remains largely underexplored due to reactivity mismatches between volatile pnictogens and the refractory components. Here, we present a predictive framework combining high-throughput machine learning-guided DFT calculations, unconventional synthesis pathways, and in situ characterization to accelerate the discovery of rare earth silicon pnictides, Ln-Si-Pn (Ln = La, Ce; Pn = P, As). Leveraging arc-melted precursors and molten salt fluxes, we alter reaction pathways to overcome synthetic barriers inherent to traditional solid state approaches. We leverage variable temperature in situ X-ray diffraction to understand complex phase dynamics within the LnSiPn3 system and guide ex situ exploration of new DFT-predicted low-energy metastable La-Si-P ternary compounds. Further, exploratory synthesis of quaternary La-M-Si-Pn (M = Mn, Au) revealed several complex structures in which incorporation of transition metals tunes the Si-P backbone connectivity. We will discuss the synthesis, structure, and properties of these multinary rare earth silicon pnictides, demonstrating how integrated workflows may enable the rational design of quantum materials.

Thursday 10:00 – 10:20 AM: From Bulk Transition Metal Dichalcogenides to Monolayers, The Intercalated Way

Presenter: Shannon Lee, Pacific Northwest National Laboratory

Kaia Brathwaite, Department of Chemistry, Xavier University of Louisiana, New Orleans LA,
Dan Thien Nguyen, Physical Sciences Division, Pacific Northwest National Lab, Richland WA,
Ajay Karakoti, Physical Sciences Division, Pacific Northwest National Lab, Richland WA,
Chih-Feng Wang, Physical Sciences Division, Pacific Northwest National Lab, Richland WA,
Andrew Ritchhart, Physical Sciences Division, Pacific Northwest National Lab, Richland WA,

Transition metal dichalcogenides (TMDs) are crucial for microelectronics and emerging quantum phenomenon but are extremely difficult to reliably produce large monolayer flakes with tunable

defects. Our systematic study of bulk crystal growth of intercalated phases, such as KxWS2, allows for simple processing of water reactive intercalants that is as simple as shaking in solution (no need for sonication or acid washes). We probe the solid state methodologies (e.g., in-situ variable temperature powder X-ray diffraction) to synthesize large bulk crystals of alkali-intercalated materials to be processed with our new method. Furthermore, once monolayers have been processed and characterized via X-ray diffraction and optical spectroscopies, we are developing an AI-guided platform in which to neatly and precisely stack new heterostructure materials.

Thursday 11:20 – 11:40 AM: Defect-Mediated Structural Transformations in Electrodeposited Nickel during Thermal Annealing

Presenter: Hyoju Park, Pacific Northwest National Laboratory

Sampreeti Bhattacharya, Pacific Northwest National Laboratory
Jack R. Grimm, Pacific Northwest National Laboratory
Kelly White, University of Minnesota

Defect engineering provides a versatile strategy for controlling the structure and properties of metallic materials for catalytic and energy applications. In metals, lattice distortions, planar defects, dislocations, and phase transformations can modify local electronic states and surface adsorption behavior, offering opportunities to enhance hydrogen-related catalytic reactions. Electrodeposition is particularly attractive for creating such nonequilibrium defect structures; however, the thermal stability and transformation pathways of electrodeposited defects remain poorly understood. In this work, defect-rich nickel thin films are fabricated by rapid electrodeposition, and their structural evolution during heating is investigated using in situ transmission electron microscopy. The results demonstrate that phase evolution is governed by defect architecture rather than temperature alone. Localized, sink-connected defects undergo recovery and rearrangement, including the formation of 9R-like interfacial structures, whereas larger and more constrained stacking-fault networks promote an fcc-to-hcp-like stacking transformation. Partial reversion during cooling highlights the metastable nature of this defect-mediated transition. Energetic modeling of fcc structures containing interfacial and stacking defects, 9R-like configurations, and hcp stacking further shows that structural stability depends strongly on defect volume fraction and spatial arrangement. Small energy differences between competing configurations facilitate transformation between them. These findings establish defect architecture as a key determinant of phase evolution in metal. Rapid electrodeposition thus provides not only a means of increasing defect density, but also a route to producing metastable structural precursors with tunable thermal behavior. The work links electrochemical growth conditions with defect-mediated phase stability and provides a framework for designing materials with controllable structures and functional properties.

Thursday 11:40 – 12:00 PM: Atom Probe Tomography of Coated 316 Stainless Steel Cladding: Mapping Elemental Distribution at Grain Boundaries

Presenter: Francelia Sanchez, Pacific Northwest National Laboratory

Sampreeti Bhattacharya, Pacific Northwest National Laboratory
Dallin Barton, Pacific Northwest National Laboratory
Jaqueline Royer, Pacific Northwest National Laboratory
Jack R. Grimm, Pacific Northwest National Laboratory
Venkata Bhuvaneswari Vukkum, Pacific Northwest National Laboratory
David Senor, Pacific Northwest National Laboratory
Arun Devaraj, Pacific Northwest National Laboratory

Defect engineering provides a versatile strategy for controlling the structure and properties of metallic materials for catalytic and energy applications. In metals, lattice distortions, planar defects, dislocations, and phase transformations can modify local electronic states and surface adsorption behavior, offering opportunities to enhance hydrogen-related catalytic reactions. Electrodeposition is particularly attractive for creating such nonequilibrium defect structures; however, the thermal stability and transformation pathways of electrodeposited defects remain poorly understood. In this work, defect-rich nickel thin films are fabricated by rapid electrodeposition, and their structural evolution during heating is investigated using in situ transmission electron microscopy. The results demonstrate that phase evolution is governed by defect architecture rather than temperature alone. Localized, sink-connected defects undergo recovery and rearrangement, including the formation of 9R-like interfacial structures, whereas larger and more constrained stacking-fault networks promote an fcc-to-hcp-like stacking transformation. Partial reversion during cooling highlights the metastable nature of this defect-mediated transition. Energetic modeling of fcc structures containing interfacial and stacking defects, 9R-like configurations, and hcp stacking further shows that structural stability depends strongly on defect volume fraction and spatial arrangement. Small energy differences between competing configurations facilitate transformation between them. These findings establish defect architecture as a key determinant of phase evolution in metal. Rapid electrodeposition thus provides not only a means of increasing defect density, but also a route to producing metastable structural precursors with tunable thermal behavior. The work links electrochemical growth conditions with defect-mediated phase stability and provides a framework for designing materials with controllable structures and functional properties.

Thursday 1:40 – 2:00 PM: Investigation of Solid-State Electrolyte Interfaces with Surface-Sensitive DNP-NMR

Presenter: J. David Bazak, Pacific Northwest National Laboratory

Dan Thien Nguyen, Pacific Northwest National Laboratory
Casey S. Mezerkor, University of Oregon, Pacific Northwest National Laboratory
Khusboo Rana, Qblox

While the advent of promising solid-state electrolyte (SSE) materials for all-solid-state batteries has been heavily driven by the search for high ionic conductivities necessary for suitable electrochemical performance, the particle surface compositions, site coordination, and reconstruction with processing and cycling is equally crucial for both engineering strategies and the elucidation of degradation mechanisms. Surface-sensitive and -selective NMR, made possible with dynamic nuclear polarization (DNP), is an emerging tool for this interfacial characterization, furnishing the means to contrast the strain, under-coordination, and functionalization of the surface sites with the conventional spectra produced by the bulk interior, even in amorphous and heterogeneous interphases. In this study, the NASICON-type ceramics M_{1+x}Al_{x}Ti_{2-x}(PO4)_{3} (M = Li, Na; LATP and NATP, respectively) are contrasted across a range of conditions and DNP polarization media. This materials class possesses relatively high ionic conductivities and intrinsic chemical stabilities (especially compared with other promising SSE families), but it is also an excellent model system for magnetic resonance techniques, with both the mobile ions and the framework being comprised of "NMR-friendly" nuclei. The investigation follows the evolution of 7Li, 23Na, 27Al, and 31P surface line shape distributions of NATP and LATP from the pristine nanoparticles to sintered pellets, with both aqueous and non-aqueous polarization media. This demonstrates how DNP can be harnessed to assess the reactive sites and surface reconstruction, correlating to material processing conditions and device performance.

Thursday 2:00 – 2:20 PM: Physical vapor deposited thin films as model systems for batteries
Presenter: Celeste Melamed, University of Oregon

Rachel Galfo, University of Oregon
Fischer Harvel, University of Oregon
Levi Hoogendoorn, Stanford University
Xin Xu, Stanford University
Stephen Kang, Stanford University
William Chueh, Stanford University

To deploy next-generation battery materials such as solid-state electrolytes and earth-abundant Na-ion cathodes, it is crucial to build a mechanistic understanding of crystalline structure during cycling. Yet batteries are heterogeneous across length scales, and complexities from additives, interfaces, and contaminants often mask the underlying solid-state chemistry. Physical vapor deposited thin films offer a uniquely powerful model system to study structure, ionics, and interfacial evolution due to precise dimensionality control, tunable crystallinity and morphology, and the availability of large-area interfaces for operando measurements. However, films are understudied for batteries due to the volatility and air-sensitivity of Li- and Na-containing materials. In this talk, we will first discuss synthesis of thin-film solid state batteries combining a LiPON solid electrolyte with lithium titanate and lithium metal electrodes, focusing on synthetic lessons learned and how thin film battery geometries can enable new insights into thermodynamics. We will next preview our recent

experiments using layered dichalcogenide thin films as a model system to probe solvent co-intercalation with high resolution X-ray diffraction techniques. To close, we will discuss the outlook for the use of physical vapor deposited thin films for battery materials.

Thursday 2:20 – 2:40 PM: From Electrolyte to Anode: Interfacial Reaction Pathways and Ion Transport in Sodium Solid State Batteries

Presenter: Dan Thien Nguyen, Pacific Northwest National Laboratory

Carinna Lapson, University of Oregon
J. David Bazak, Pacific Northwest National Laboratory
Shannon J. Lee, Pacific Northwest National Laboratory

The development of solid-state sodium batteries demands electrolytes that conduct Na^+ efficiently while withstanding the harsh reductive environment of low-potential anodes. We prepared phase-pure Cl-doped Na3PS4 (c-NPSC), confirmed in the cubic phase by ^{23}Na magic angle spinning nuclear magnetic resonance and X-ray diffraction, with an ionic conductivity of 0.7 mS cm-1. We investigated the c-NPSC/Na9Sn4 interface by X-ray photoelectron spectroscopy (XPS) and operando electrochemical impedance spectroscopy (EIS) with distribution-of-relaxation-times (DRT) analysis. Below 0.1 V vs. Na9Sn4, XPS detected potential-dependent metal sulfide and phosphide deposits from reductive c-NPSC decomposition. DRT decomposed the impedance into four contributions: bulk conduction, interphase resistance, charge transfer, and diffusion (τ = 10-6–10 s), with total resistance growing by less than 10% over 17 hours. Against a TiS2 cathode at 0.05 mA cm-2, full cells retained 99.95% Coulombic efficiency across 50 cycles, confirming c-NPSC electrolyte promotes a self-passivating, ion-conducting interphase.

Thursday 3:00 – 3:20 PM: Femtosecond laser ablation (fs-la) - a new approach to XPS depth profiling

Presenter: James Lallo, Thermo Fisher Scientific

Tim Nunney, Thermo Fisher Scientific
Mark Baker, University of Surrey

X-ray Photoelectron Spectroscopy (XPS) depth profiling is a widely used analytical technique for determining the chemical composition and chemical state distribution within thin films, coatings, multilayer structures, and engineered materials. Conventional XPS depth profiling relies on ion beam sputtering, which can induce significant chemical damage and preferential sputtering effects in many organic and inorganic materials, complicating the interpretation of depth-dependent chemical information. The Thermo Scientific™ Hypulse™ XPS introduces femtosecond laser ablation as a complementary material removal technique for XPS depth profiling. By minimizing the chemical and structural modifications commonly associated with ion beam sputtering, femtosecond laser ablation enables the characterization of a broad range of challenging materials while providing access to significantly greater analysis depths and faster profiling rates. This presentation will focus

on the practical application of Hypulse XPS for the characterization of advanced materials relevant to energy storage, catalysis, and functional materials research. Examples will include depth-resolved analysis of battery materials such as graphite-silica composite anodes, lithium fluoride-containing interfaces, and coated NMC cathode particles, where preservation of chemical information is critical to understanding material performance. Additional case studies will demonstrate the analysis of complex transition metal oxides and large organometallic compounds that are difficult to characterize using conventional sputter-based depth profiling approaches. These examples highlight how femtosecond laser ablation XPS expands the range of materials accessible to depth-resolved chemical analysis and provides new opportunities for investigating complex, heterogeneous materials systems. The capabilities of the Hypulse XPS platform and its potential impact on advanced materials characterization will be discussed.

Thursday 3:20 – 3:40 PM: Developments in sample preparation, loading, and pre-analysis treatment for Cryo-XPS of volatile and soft materials.
Presenter: Chris Moffitt, Kratos Analytical

Jonathan Counsell, Kratos Analytical
Liam Soomary, Kratos Analytical

Utilization of XPS continues to increase in traditional materials analysis, as well as expanding into disciplines that previously were limited in their use of surface analysis. Much of this expansion has been the result of equipment developments in recent years, with new technologies, such as gas cluster ion sources allowing for the etching of soft materials.

Thursday 3:40 – 4:00 PM: Reconfigurable Automation Carts: Ginkgo Bioworks' Modular RACs Provide Throughput and Flexibility in Autonomous Labs
Presenter: Daniel Curhan, Ginkgo Bioworks

Imagine an organization where any scientist, at any time, from any desk (or couch or plane), can conjure an experiment, and simply describe it in words to their autonomous lab. The lab then automatically runs their scientific protocol, and delivers trustworthy, consistent, traceable results immediately when the protocol finishes. Imagine this service running 24 hours a day, seven days a week, staffed not by human pipettors trapped at their lab benches, but by robots, conveyors, and automated liquid handlers. If it's this easy for one scientist to turn an idea into real experimental data, imagine how many experiments that one scientist can run. Imagine how much data a team of scientists can generate. This is the lab of the future.

Thursday 4:40 – 5:00 PM: Understanding ethylene selectivity for ethane oxidation on Cl-substituted IrO2(110) through microkinetic modeling

Presenter: Jungwon Yun, University of Florida

Connor Pope, University of Florida
Minkyu Kim, Yeungnam University
Jason Weaver, University of Florida
Aravind Asthagiri, The Ohio State University

Selective ethylene production from ethane oxidation is an attractive alternative to energy-intensive steam cracking. However, alkane activation requires high temperatures, and thermodynamics favor complete oxidation. Previous temperature-programmed reaction spectroscopy (TPRS) and density functional theory (DFT) studies showed that stoichiometric IrO2(110) facilitates C-H bond activation of light alkanes at low temperatures. Predosing hydrogen to form surface hydroxyl (HO) groups improved ethylene selectivity by blocking sites for further dehydrogenation and oxidation. Because chlorine (Cl) is isoelectronic with HO, we investigated Cl substitution at Obr sites. DFT calculations show that adjacent Cl atoms destabilize adsorbed ethane and ethylene while minimally affecting C-H bond cleavage barriers, suggesting that partial Cl substitution preserves ethane activation while suppressing overoxidation. We developed a DFT-based microkinetic model (MKM) to study ethane conversion and product yields varied by Cl coverage. A conventional mean-field MKM failed to produce ethylene due to the low dehydrogenation barriers. To address this limitation, we incorporated surface diffusion-limited kinetics, where diffusion barriers increase the effective activation energy for dehydrogenation. The revised model predicts nearly 100% ethylene yield at ~0.4 Cl surface coverage, whereas TPRS experiments measured only ~30%, indicating missing oxidation pathways. Additional DFT calculations identified a low-barrier (~90-100 kJ/mol) hydrogen-hopping pathway converting unreactive HObr to reactive Obr atoms near C2Hx intermediates, promoting oxidation over ethylene desorption. Incorporating this step into the MKM significantly improved the agreement with experiments, identifying surface hydrogen-hopping as a key factor governing ethylene selectivity. Future work will examine Cl-substituted IrO2(110) under steady-state reaction conditions at higher pressures.

Friday 8:40 – 9:00 AM: Co-Adsorption of Acetic Acid with H2O on Anatase TiO2(101)

Presenter: Joshua Wagner, Pacific Northwest National Lab

Zbynek Novotny, PNNL
Zdenek Dohnalek, PNNL

The adsorption geometry of carboxylic acids on metal oxides controls key steps in ketonization. While molecular and deprotonated binding modes of acetic (and formic) acid on anatase TiO2(101) are known, how co-adsorbed water influences adsorption, proton transfer, and surface mobility on this facet remain unclear. Here, we combine angle- and energy-resolved molecular beam scattering

with scanning tunneling microscopy to probe acetic-acid binding motifs in the presence of water on anatase TiO2(101). Molecular scattering addresses energy-transfer dynamics for the adsorption of acetic acid dimers, and STM tracks water-mediated ordering, the dissociation of dimers, and deprotonation of individual acetic acid molecules across terrace and step sites on anatase titania's most stable crystal face. Overall, this work provides a molecularly resolved description of the dynamics governing the formation of acetate intermediates in the presence of water on a-TiO2(101) with results relevant for ketonization on metal oxides.

Friday 9:00 – 9:20 AM: Site-Specific Deuterium Adsorption in Nitrogen-Doped Graphene and Porous Carbon Materials

Presenter: Zbynek Novotny, Pacific Northwest National Laboratory

Buddhika S. Alupothe Gedara, Pacific Northwest National Laboratory
Peter S. Rice, Pacific Northwest National Laboratory
Tom Autrey, Pacific Northwest National Laboratory
Bojana Ginovska, Pacific Northwest National Laboratory
Mi Yeon Byun, Pacific Northwest National Laboratory
Zdenek Dohnálek, Pacific Northwest National Laboratory

Nitrogen-functionalized carbon materials are investigated as promising candidates for hydrogen activation and storage. We investigated three model systems: N-doped highly-oriented pyrolytic graphite (N-HOPG), N-doped graphene/Ru(0001), and porous nitrogen-carbon (NC) synthesized by pyrolysis of glucose and graphitic carbon nitride. For the first two systems, a variable N concentration was introduced using ion irradiation. Nitrogen incorporation occurs preferentially in two configurations: graphitic N (GN; N substituted in the hexagonal C lattice), and pyridinic N (PN; substitutional N adjacent to a C vacancy). The relative concentrations of GN and PN can be controlled by varying the ion dose, annealing temperature, and the choice of substrate. For all probed materials, X-ray photoelectron spectroscopy showed that D exposure induces a shift of the PN peak to higher binding energy, while the GN peak remains unchanged, demonstrating that deuterium binds selectively to PN sites. A near complete saturation of PN sites with D atoms was observed for N-HOPG. Only a partial saturation of PN sites was observed for N-doped graphene/Ru(0001) (due to the necessity to cleave the N-Ru bond before D adsorption) and in porous NC (consequence of limited accessibility due to pore confinement effects). Deuterium fully desorbed from N-HOPG above 900 K, whereas on N-doped graphene/Ru(0001), a complete D desorption from PN is observed at ~700 K, indicating that the Ru metal weakens the N-D bond strength. Moreover, the NC exhibited nearly the same desorption behavior as N-HOPG, demonstrating that well-defined model systems can effectively capture the behavior of more complex N-doped carbon materials.

Friday 9:20 – 9:40 AM: Influence of Substrate Interactions on the Growth of MoO3 on Graphene/Ru(0001) and Highly-Oriented Pyrolytic Graphite

Presenter: Buddhika Alupothe Gedara, Pacific Northwest National Laboratory

Zdenek Dohnalek, Pacific Northwest National Laboratory
Zbynek Novotny, Pacific Northwest National Laboratory

Molybdenum trioxide (MoO3) stands out for its high dielectric constant, wide band gap, and catalytic activity, enabling diverse electronic and energy-related applications. In this work, we investigate the effects of substrate topography and charge transfer on MoO3 growth on HOPG and graphene (Gr)/Ru(0001) using scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). Upon increasing the temperature to 500-700 K, more ordered, crystalline MoO3 islands form on both substrates. Notably, a distinct height difference of MoO3 is observed on these two substrates over the studied temperature range. The height of MoO3 islands on Gr/Ru(0001) corresponds to a single layer of MoO3 (3.9 Å), whereas the height of the MoO3 islands on HOPG is consistent with the previously reported double layer (6.8 Å). Additionally, we observed a brick-style pattern on the MoO3 islands on Gr/Ru(0001) substrate and the formation of this characteristic pattern is due to the ordered removal of terminal oxygen atoms. XPS data show that Mo in the islands on HOPG are predominantly in (6+) oxidation state while on Gr/Ru(0001) at least half is reduced to (5+) over the temperature range of 500-700 K. The formation of lower oxidation states is attributed to charge transfer from the substrate due to the electron chemical potential difference at the interface, and the presence of oxygen vacancies. Our results demonstrate that substrate-induced interfacial interactions play a key role in controlling the nucleation and growth mode.

Friday 10:40 – 11:10 AM: Freestanding Metal Film Device Platform for In Situ Electron Magnetic Circular Dichroism and Hall-Voltage Measurements

Presenter: Libor Kovarik, Pacific Northwest National Laboratory

Charge-neutral Hall effects, such as the spin Hall effect and orbital Hall effect play a central role in spintronics and information transport. Recent developments indicate that electron magnetic circular dichroism (EMCD) in scanning transmission electron microscopy (STEM), performed under electrical bias, may provide a route for directly probing Hall-current-induced spin and orbital accumulations with nanometer-scale resolution. However, realizing this emerging capability requires specimens that satisfy stringent structural and geometrical conditions under in-situ electrical bias. We introduce a method for preparing and integrating free-standing metallic films for in-situ EMCD measurements of Hall transport phenomena. The films are grown by molecular beam epitaxy, released from their substrates using water-soluble sacrificial layers, transferred onto biasing chips and patterned by focused ion beam. Two device architectures are developed: a simple-bridge configuration for current-driven EMCD measurements and a cross-bridge configuration additionally enabling conventional Hall voltage measurement. The developed platform is demonstrated for Ni

and Cr films and validated by reliably reproducing the metal's characteristic Hall responses, while EMCD spectra acquired from ferromagnetic Ni validate compatibility with magnetic dichroism measurements. The platform provides a new route for nanoscale studies of charge-neutral Hall effects in STEM, enabling direct correlation of local electronic structure, microstructure and transport properties.

Friday 11:10 – 11:40 AM: Evolution of Aerosol Properties from Ground to Aloft: Physicochemical Changes, Phase Behavior, and Cloud Interactions

Presenter: Nurun Nahar Lata, Pacific Northwest National Laboratory

Zezhen Cheng, Pacific Northwest National Laboratory
Darielle Dexheimer, Sandia National Laboratory
Swarup China, Pacific Northwest National Laboratory

The physicochemical properties of atmospheric aerosols evolve as particles are transported, mixed, and processed under changing environmental and meteorological conditions. Changes in morphology, composition, mixing state, and phase state can influence particle behavior and interactions with clouds. However, how these properties evolve with altitude and under different atmospheric conditions remains poorly constrained, in part because most observations are made near the surface and bulk measurements cannot fully capture the diversity of individual particles. To address this gap, aerosol samples were collected at ground level and aloft during several U.S. Department of Energy field campaigns using a size- and time-resolved aerosol collector (STAC) to examine aerosol evolution across contrasting environments. Computer-controlled scanning electron microscopy with energy-dispersive X-ray spectroscopy (CCSEM/EDX) and scanning transmission X-ray microscopy with near-edge X-ray absorption fine structure spectroscopy (STXM/NEXAFS) were used to determine particle morphology, elemental composition, carbon speciation, and mixing state. These measurements revealed clear differences between near-surface and elevated aerosol populations in composition, mixing state, and phase behavior, with additional changes associated with cloud processing and cold, humid conditions. Such vertical variability can alter particle water uptake and cloud-relevant behavior, highlighting the limitation of relying on ground-based observations alone. Together, these observations connect aerosol sources, meteorological conditions, and atmospheric processing with changes in particle properties and provide a more complete picture of how aerosols evolve from the ground to aloft and how that evolution influences cloud interactions.

Friday 11:40 – 12:00 PM: Multifunctional Peptoid Nanomembranes for Chemical Agent Degradation and Antiviral Applications

Presenter: Thi Kim Hoang Trinh, Pacific Northwest National Laboratory

Baylie Phillips, Department of Materials Science and Engineering, University of Washington, Seattle, WA 98195, USA
Xiaojie Lin, Department of Materials Science and Engineering, University of Washington, Seattle, WA 98195, USA
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Emerging chemical and biological threats pose persistent public health and global security challenges because of their toxicity, rapid evolution, and potential for widespread impact.1 Existing technologies often lack the adaptability and specificity required to address these threats, highlighting the need for scalable, programmable countermeasures. Peptoids (poly-N-substituted glycines) are sequence-defined polymers that self-assemble into hierarchical, crystalline nanomaterials through noncovalent interactions.2-3 Their structures and functions can be precisely tuned through side-chain modification and co-assembly, making them attractive for catalysis,4 sensing,5 antiviral therapies,6 and mineralization.7 Here, we develop peptoid-based crystalline assemblies as a programmable platform for degrading chemical warfare agent (CWA) simulants and inhibiting viruses. We created active peptoid nanomembranes by incorporating metal ions, bioactive molecules, or nanoparticles as surface-bound active sites with controlled alignment and density. These functionalities were introduced through N-terminal modification during solid-phase synthesis or after assembly. The rotational chemistry of peptoid building blocks also generates enzyme-like microenvironments that promote catalytic activity. Accordingly, membranes containing metal complexes or nanoparticles hydrolyzed CWA simulants into benign products under mild, ambient conditions. Membranes functionalized with bioactive molecules that mimic viral binding receptors inhibited multiple viral pathogens, including Influenza A (H1N1) and Sindbis virus. These results demonstrate that peptoid assemblies provide a versatile and programmable materials platform for simultaneously addressing chemical and biological threats.

Graduate Students Posters

GS1. Morphology control enables Electrowinning from inactive FeOx at fast rates

Presenter: Raj Shekhar, University of Oregon

Shannon Boettcher, University of California, Berkeley
Paul Kempler, University of Oregon

Previous investigations on low-temperature iron electrowinning have considered the material phase as the key factor that influences the reduction kinetics. Recent results suggest that the nanoscale morphology of the iron-oxide can also have a substantial effect on the reactivity. However, the relative influence of phase and morphology have not been established. Here, we showed that nanoscale morphology dominates the reduction kinetics over the phase of iron oxide. In this study, we investigated the electrochemical behavior of magnetite and hematite nanoparticles with similar morphologies and found that both exhibit identical kinetics, with a faradaic efficiency of nearly 80%. Using thin-film rotating ring-disk measurements, we discovered that both magnetite and hematite undergo reductive dissolution, however, magnetite reduction is influenced by surface passivation, whereas hematite is not. We also found that the amount of soluble ferrous intermediates produced can predict metal deposition efficiency in model electrowinning setups. Based on these findings, inactive blast furnace iron-oxide powders (7%, faradaic efficiency) were converted into high surface area nanoparticles (60%, faradaic efficiency) via a reprecipitation route. This process achieved a partial current density towards iron electrowinning in excess of 120 mA cm-2, which is among the highest reported value for low-temperature iron electrowinning from inactive oxide ores. In summary, these results indicate the importance of morphology to activate industrial iron oxides and highlight that phase identity itself is not sufficient to predict electrochemical iron production performance. Therefore, natural ores require morphological changes to be economically viable for the industrial electrowinning.

GS 2. Anion-Induced Solvation Effects on Charge Storage Competition in Aqueous Mg-Ion Prussian Blue Cathode

Presenter: Micah Wilson, Oregon State University

Mason Lyons, School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, Oregon 97331
Zachary Regan, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331
Logan Lancaster, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331,
Taylor Krueger, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331
Isabelle Logan, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331

Xiulei Ji, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331
Chong Fang, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331
Zhenxing Feng, School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, Oregon 97331

Aqueous magnesium ion batteries represent a promising technology for large-scale energy storage due to the natural abundance of magnesium, its high multivalent charge density, and the compatibility of magnesium metal with aqueous electrolytes. However, the strong hydration shell of Mg2+ impedes ion transport kinetics and intercalation, even in cathode materials with large interstitial sites such as iron hexacyanoferrate (FeHCF, Prussian Blue). Here, we demonstrate that Hofmeister anion effects provide a molecular-level strategy to tune electrolyte solvation structure and thereby control the dominant charge-storage mechanism in FeHCF. Using saturated MgSO4, MgCl2, and Mg(ClO4)2 electrolytes spanning the kosmotropic to chaotropic range of the Hofmeister series, femtosecond simulated Raman spectroscopy and 25Mg NMR reveal that the kosmotropic SO42- anion reinforces an extended hydrogen-bonding network and perturbs the Mg2+ solvation shell, whereas the chaotropic ClO4- anion disrupts the hydrogen-bonding network and preserves the Mg2+ solvation shell, while Cl- exhibits intermediate behavior. These distinct solvation environments directly govern electrochemical charge storage. FeHCF cycled in saturated MgSO4 delivers an initial specific capacity of 70 mAh g-1 through predominantly Grotthuss proton charge transfer, whereas Mg(ClO4)2 and MgCl2 support direct Mg2+ intercalation, delivering lower capacities of 45 and 43 mAh g-1, respectively. Galvanostatic cycling, GITT, EQCM, and post-cycling structural characterization consistently support this transition from proton to magnesium dominated charge compensation across the Hofmeister series. Together, these findings establish a clear design principle linking anion properties, solvation structure, and charge storage mechanism in aqueous multivalent batteries.

GS 3. Area-Selective Deposition of Tungsten Oxide

Presenter: Kylee Lamberson, Oregon State University

Brian Muhich, Oregon State University
Changqing Pan, Oregon State University
Chih-hung Chang, Oregon State University

We grew thin films of tungsten oxide (WO3) on different seed materials using a custom-built atomic layer deposition chamber. Tungsten carbonyl (W(CO)6) and water (H2O) were used as precursors for the deposition of WO3. Tetraethyl orthosilicate (TEOS) was used in a batch method to synthesize the silica (SiO2) seed material. Titanium(IV) isopropoxide (TTIP) was used as a precursor in a custom-built vapor-phase microreactor-assisted nanomaterial deposition (V-MAND) system to synthesize and deliver titania (TiO2) particles. Both seed materials were deposited on polyimide and silicon substrates. The selectivity window was investigated for depositing WO3 on these seed materials vs the nongrowth areas of the substrates. Scanning electron microscopy (SEM) was used to measure

seed material particle sizes and energy-dispersive x-ray spectroscopy (EDX) to confirm their composition. Laser ablation laser ionization time of flight mass spectrometry (LALI-TOF-MS) was used to map the selectively deposited areas. Results are still being finalized.

GS 4. Composition Engineering of $SrCo_{1-x}Ir_xO_3$ Perovskite Electrocatalysts for Acidic Oxygen Evolution

Presenter: Saowaluk Soonthornkit, Oregon State University

Zhenxing Feng, School of Chemical, Biological, and Environmental Engineering, Oregon State University
Kai Shen Choong, School of Chemical, Biological, and Environmental Engineering, Oregon State University

Hydrogen produced from proton exchange membrane water electrolysis (PEMWE) is a promising pathway toward sustainable energy conversion and storage. However, the sluggish kinetics of the oxygen evolution reaction (OER) and the reliance on iridium-based catalysts limit the large-scale deployment of PEMWE. Developing electrocatalysts that reduce iridium content while maintaining high activity is therefore essential. In this work, the Co/Ir composition of $SrCo_{1-x}Ir_xO_3$ (SCIO) perovskite catalysts was systematically varied to investigate the influence of composition on acidic OER performance. A series of SCIO catalysts with different Co ratios were synthesized via a sol-gel method and evaluated using rotating disk electrode (RDE) measurements in acidic electrolyte and a laboratory-scale PEM electrolyzer. Structural and surface characterization was performed using X-ray diffraction (XRD), while X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) will be discussed to provide insight into the electronic structure and local coordination environments associated with the composition-dependent catalytic performance. This study demonstrates the potential of composition engineering to reduce iridium content while maintaining efficient OER activity, offering guidance for the development of cost-effective perovskite electrocatalysts for PEM water electrolysis.

GS 5. Energetics of Water Adsorption on H- and CO-Precovered Pt(111) Surfaces: Solvent – Adsorbate Interactions

Presenter: Arjan Saha, Washington State University

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

Carbon monoxide (CO) and hydrogen (H2) are widely studied adsorbates in surface science and catalytic processes. Here, we employ single-crystal adsorption calorimetry (SCAC) and sticking coefficient measurements to investigate how preadsorbed H- and CO- influence the interaction of Pt(111) with the prototypical solvent water (D_2O). At 100 K, the initial sticking probability of D_2O on CO/Pt(111) is high (~0.9) and increases asymptotically to unity with coverage. The heat of adsorption remains constant over submonolayer coverages and equals the multilayer value, suggesting weaker D_2O binding to CO/Pt(111) than to bare Pt(111). Increasing the temperature to 130 K decreases the initial sticking probability to ~0.2. At higher coverages, sticking approaches unity only well above 1 ML, indicating three-dimensional D_2O cluster formation and non-wetting behavior. H_2 pre-exposure produces ~0.8 ML of dissociated hydrogen on Pt(111). At 100 K, the initial D_2O sticking probability on H/Pt(111) is ~0.7 and increases to unity with coverage. Adsorption follows a hit-and-stick mechanism, with decreased monolayer sticking probabilities and a heat of 45 kJ/mol, indicating a disordered, metastable monolayer. At 140 K, thermally activated surface mobility restores ordered layer-by-layer growth with initial sticking probability at ~0.7 increasing to unity with coverage, and the adsorption heats initially at 43 kJ/mol and subsequently increasing to the 48 kJ/mol multilayer value. These results show the modification of coadsorbed species in solvent binding and growth on Pt(111) by controlling adsorption energetics, molecular mobility, hydrogen bonding, and water growth morphology.

GS 6. Influence of Surface Finish on Electrochemical Performance of ALD Corrosion Barriers on Additively Manufactured SS316L

Presenter: Noah Montrose, Boise State University

Brandon King, Boise State University
Julie Li, Boise State University
Dr. Mike Hurley, Boise State University

Metal additive manufacturing via laser powder bed fusion (LPBF) enables rapid production of complex components to improve Naval fleet readiness. While stainless steel 316L (SS316L) is favorable for marine applications due to its self-healing native oxide film, LPBF processing introduces defects like high surface roughness, micro-cracking, and elemental segregation which can accelerate localized corrosion. This study investigates the feasibility of 100nm atomic layer deposition (ALD) alumina and titania thin films as corrosion-mitigating barriers, focusing on understanding the impact of substrate surface morphology. To evaluate these effects, ALD films were deposited onto two distinct substrate conditions: as-printed LPBF and LPBF polished to 600-grit, with wrought SS316L used as a benchmark. Electrochemical characterization was performed in 0.6M NaCl to evaluate the properties of the passive film before and after induced polarization. Electrochemical impedance spectroscopy and equivalent circuit fitting were used to model and quantify the coating properties of the protective barrier using Bode plots and equivalent circuit values. Cyclic potentiodynamic polarization was used to characterize the passive behavior and breakdown

potentials of the coated samples. Additionally, Mott-Schottky experiments evaluated the semiconducting properties of the protective films, allowing for the determination of carrier densities and flat-band potentials. Initial results demonstrate that the presence of an ALD coating led to enhanced passivity and a decrease in the corrosion current density. The low-frequency impedance values for the alumina film were approximately three orders of magnitude greater than the uncoated and titania specimens, which exhibited comparable performance.

GS 7. First-Principles Investigation of Water Activation on Rh Single-Atom Catalysts Supported on Fe_3O_4(001)

Presenter: Chukwuma Ndive , Pacific Northwest National Laboratory

Benjamin A. Jackson, Pacific Northwest National Laboratory
Daniel Baranowski, Pacific Northwest National Laboratory
Liney Arnadottir, Oregon State University; Pacific Northwest National Laboratory
Zbynek Novotny, Pacific Northwest National Laboratory
Mal-Soon Lee, Pacific Northwest National Laboratory
denek Dohnalek, Pacific Northwest National Laboratory

Single-atom catalysts (SACs) provide isolated, highly active metal centers and the support plays an important role in influencing the stability and activity of single atoms. Water activation is a fundamental step in heterogeneous catalysis, therefore, understanding the mechanism of water interaction on oxide surfaces at the atomic scale is essential for improved catalyst design. Here, periodic density functional theory calculations are performed for a Rh/Fe3O4(001) slab model to investigate the mechanism of water adsorption, deprotonation, and hydroxyl recombination on Rhad and Rhoct. Water dissociation barriers are obtained for Rhad(H2O)n=1-2 complexes involving protonation of lattice oxygen at tetrahedral Otet or bulk-like open OBLO surface sites. Water adsorption is more favorable on Rhad with a binding energy of -1.33 eV than on Feoct with -0.73 eV. Different water binding motifs, namely pseudo-square planar, square planar and octahedral, were observed. The adsorbed water oxidizes the Rh atom, leading to a change in oxidation state as seen from the Bader charge of 0.88 e, an increase of 0.33 relative to the bare two-fold Rh adatom. For isolated water molecules, molecular adsorption on Rh is energetically more favorable than dissociative adsorption at -1.18 eV. A Rh(H2O) protonates either of the two lattice oxygens, then a Rh(OH) protonates the lattice OH to yield a recombinative water. This is more favorable to OBLO, despite the less favorability to protonate OBLO. Our results provide atomic-scale insight into water activation and recombination on Rh/Fe3O4(001) which would offer design principles for developing efficient oxide-supported catalysts for other sustainable energy technologies.

GS 8. Structural Influences on Solvent Co-Intercalation in Transition Metal Diselenide Thin Films

Presenter: Rachel Galfo, University of Oregon

Joseph Daddona, University of Oregon

Solvent co-intercalation is a promising strategy to enable high-rate battery charging by lowering desolvation barriers at the electrode–electrolyte interface. Previous studies have largely focused on the effects of electrolyte composition, solvent coordination strength, and salt concentration, whereas comparatively little attention has been given to how the host structure and interlayer environment govern solvent uptake and transport. Further, conventional carbonate electrolytes are generally treated as non-co-intercalating systems because formation of a solid electrolyte interphase suppresses solvent insertion in conventional layered electrodes. Consequently, the structural characteristics that enable reversible carbonate-solvent co-intercalation remain poorly understood. Here, we investigate solvent co-intercalation in turbostratic 1H-$NbSe_2$ and 1T-VSe_2 thin films synthesized by electron-beam physical vapor deposition using the modulated elemental reactants method. Although both materials are metallic, 1H-$NbSe_2$ and 1T-VSe_2 possess distinct layered crystal structures, with trigonal-prismatic and octahedral metal coordination, respectively. These differences provide a model system for examining how the host crystal structure and electronic properties influence solvent-assisted ion insertion. Electrochemical behavior in a conventional carbonate electrolyte is compared with that in a co-intercalating diglyme electrolyte. In both host structures, carbonate-solvent co-intercalation produces greater than 80% expansion of the layered structure, as determined by specular X-ray diffraction, X-ray reflectivity, and X-ray fluorescence measurements following electrochemical cycling. These structural measurements are correlated with electrochemical performance to evaluate diffusion coefficients, reversible capacity, and cycling stability. This work examines co-intercalation of carbonate and diglyme electrolytes in turbostratic transition-metal dichalcogenides and establishes how host crystal structure influences transport kinetics and electrochemical performance.

GS 9. Direct visualization of sacrificial layer dissolution during freestanding membrane release processes using Cryo-ToF-SIMS

Presenter: Hsin-Mei Kao, Oregon State University

Min-Ju Choi, Pacific Northwest National Laboratory
Jennifer Yao, Pacific Northwest National Laboratory
Chih-Hung Chang, Oregon State University
Peter V. Sushko, Pacific Northwest National Laboratory
Zihua Zhu, Pacific Northwest National Laboratory
Yingge Du, Pacific Northwest National Laboratory

Freestanding membranes enable transferable, strain-relaxed thin films for flexible electronics, heterogeneous integration, and advanced functional devices. Their release commonly relies on

selective wet etching of a buried sacrificial layer and is often accompanied by cracking, wrinkling, and other mechanical failures. However, most studies have focused on membrane materials and post-release transfer, leaving the interfacial mechanisms governing sacrificial-layer dissolution and membrane lift-off poorly understood. Here, we combine D2O isotopic labeling with cryogenic time-of-flight secondary ion mass spectrometry (cryo-ToF-SIMS) to characterize the buried interface during SrO dissolution in an MBE-grown Pd/SrO/LSAT(001) model system. Rapid freezing preserves the transient interfacial state, enabling ToF-SIMS to reveal three key features: web-like D2O infiltration pathways, island-like residual SrO pillars supporting the Pd membrane, and D2O-depleted regions where the SrO has been fully removed and the Pd membrane has collapsed onto the substrate. Correlative ToF-SIMS analysis and 3D optical profilometry further reveal a membrane lift height of approximately 93 ± 10 μm and a steep local lifting angle of approximately 71°. These observations demonstrate that membrane release proceeds through a highly heterogeneous interfacial process rather than a uniform dissolution front. Together, these results provide molecular and morphological insight into sacrificial-layer etching and highlight cryo-ToF-SIMS as a powerful method for uncovering otherwise inaccessible interfacial processes governing freestanding-membrane release.

GS 10. Quantifying the Impact of "29" Copper Surface Oxide Fluxionality on Single-Site Pt-Catalyzed Low-Temperature CO Oxidation

Presenter: Zhicheng Yu, Washington State University

Maura Castillo, Washington State University
Denis Sholotyuk, Washington State University
Jean-Sabin McEwen, Washington State University, Pacific Northwest National Laboratory

CO oxidation over automotive exhaust catalysts typically requires elevated temperatures because the strong adsorption of CO inhibits its activation and subsequent conversion to CO_2 under low-temperature conditions. Recently, a new structural model for the “29” copper surface oxide was proposed, and experimental studies have demonstrated enhanced low-temperature CO oxidation activity when Pt is deposited on this oxide. We have recently shown that the ground-state “29” copper surface oxide structure coexists with several alternative surface oxide configurations possessing the same stoichiometry and unit cell as the ground-state structure, whose energies lie within the uncertainty of density functional theory (DFT) calculations, implying that the surface oxide is inherently fluxional. To quantify the impact of this fluxionality on low-temperature CO oxidation, we employ the Atomistic Global Optimization X (AGOX) framework. AGOX combines global optimization with active Δ-learning and universal machine-learning potentials, enabling efficient identification of favorable Pt deposition sites across an ensemble of accessible “29” copper surface oxide structures. Our results demonstrate that support fluxionality gives rise to multiple distinct single-site Pt coordination environments, highlighting the importance of considering an ensemble of oxide structures rather than a single static model when describing catalytic behavior. We further investigate how variations in Pt location and coordination influence CO oxidation through a Mars–

van Krevelen mechanism. Minimum-energy reaction pathways are characterized using both conventional DFT calculations and universal machine-learning potentials, enabling accelerated exploration of reaction energetics while maintaining high fidelity.

GS 11. Hydrogen Dissociation and spill over for Pt single Site on CeO_2(100)

Presenter: Christian Andrade, Oregon State University

Honghong Shi, Pacific Northwest National Laboratory
Liney Arnadottir, Oregon State University

Atomically dispersed Pt on CeO2 provides unique active sites governed by its local environment while minimizing noble-metal loading. The role of CeO_2 during H_2 activation at isolated Pt sites remains unclear, particularly whether dissociated hydrogen remains on Pt or transfers to the support. Spin-polarized DFT+U calculations and transition-state searches were used to examine H_2 adsorption, cleavage, and surface migration for single-atom Pt site on stoichiometric and oxygen-deficient CeO_2(100) surfaces. Vibrational calculations further distinguish Pt–H, vacancy-associated hydrogen, and hydroxylated interfacial configurations. The calculated pathway begins with H–H cleavage over the Pt site, forming two Pt-bound hydrogen atoms. Hydrogen subsequently transfers to a neighboring lattice oxygen, forming a Pt–H/OH interfacial configuration. Reverse transfer from OH to Pt is less favorable, while migration between lattice oxygen sites provides a pathway for hydrogen redistribution across the surface. Bader charge and spin analyses identify hydride-like Pt–H character, electron localization in Ce 4f states, and reduction of neighboring Ce^{4+} centers. Overall, Pt initiates H–H cleavage, while CeO_2 accepts and redistributes the dissociated hydrogen. These results highlight the importance of the interplay between the single site, support, and the local environment.

GS 12. Fabrication and Investigation of Two-Dimensional Gold Nanosnowflakes for SERS Applications

Presenter: Annabella Talbott, Western Washington University

Ying Bao, Western Washington University

Two-dimensional branched nanostructures have previously shown promise as surface enhanced Raman spectroscopy (SERS) candidates and for catalysis. This project aims to fabricate a specific type of branched nanostructures, gold nanosnowflakes (AuNSFs), as well as investigate their growth. Using a seed-mediated method, AuNSFs are able to be rapidly grown and the conditions of the growth solution's effect on their final morphology has been studied. Their optical properties have also been investigated. Finally, their use as SERS candidates has been explored to understand the relationship between an observed signal and the local environment's structural distribution.

GS 13. Design and fabrication of sputtered amorphous silicon carbide photonic ring resonators

Presenter: Asif Bhuiyan, Boise State University

Ben Reigle, Boise State University
Karthik Srinivasan, Boise State University

Silicon photonics has established itself as a leading platform for integrated optics, owing to low propagation losses in the near-infrared (NIR) wavelengths, the availability of its native oxide to be used as cladding and similar device fabrication processes to electronics. However, silicon's narrow bandgap and thermal instability at elevated temperatures limit its performance in harsh environments, necessitating a transition toward wide-bandgap materials like silicon carbide (SiC). While crystalline SiC demonstrates exceptional optical properties—including a high refractive index, broad transparency from visible to mid-infrared wavelengths, a low thermo-optic coefficient, and strong optical nonlinearities—its monolithic integration is severely constrained by poor crystal growth on amorphous substrates like silica. Existing fabrication strategies, such as smart-cut ion-slicing or substrate under-etching, remain complex and face significant scalability and yield challenges. To address these limitations, this work explores amorphous silicon carbide (a-SiC) as a versatile, CMOS-compatible alternative that can be sputter-deposited at room temperature with more precise thickness control. We perform a rigorous spectroscopic characterization of both as-deposited and annealed a-SiC thin films to evaluate their optical properties based on which, we simulate and optimize the geometric dimensions required for single-mode waveguide operation. Finally, we report the systematic optimization of the entire fabrication pipeline—spanning film deposition, lithography, and reactive-ion etching—culminating in the successful realization of a-SiC microring resonators. This approach provides a robust, high-yield framework for extreme environment photonics.

GS 14. Stress annealed CoFeBNb Ribbons for High-Performance Electrical Applications

Presenter: Miguel Mancias, Boise State University

Nickolaus M. Bruno, Materials and Structures Division, NASA Glenn Research Center, Cleveland, Ohio, USA
Vladimir Keylin, Materials and Structures Division, NASA Glenn Research Center, Cleveland, Ohio, USA; HX5 LLC, Brookpark, OH 44135, USA
Alex M. Leary, Materials and Structures Division, NASA Glenn Research Center, Cleveland, Ohio, USA
Ronald D. Noebe, Materials and Structures Division, NASA Glenn Research Center, Cleveland, Ohio, USA
Karthik Srinivasan, Electrical and Computer Engineering, Boise State University, Boise, Idaho, USA

This work presents a continuous stress annealing process for Co60Fe20B15Nb5 (at.%) ribbons,

designed to optimize the performance of high-power soft-magnetic inductor cores and transformers for aerospace and other high-power applications. The study addresses Co-based alloy processability tackling the competing demands of high saturation induction, Bsat, and low coercivity, Hc, in magnetic materials, which are critical for achieving high-power density and energy efficiency. To achieve this, a strong longitudinal magnetic anisotropy was induced through stress annealing of the ribbon using a high-throughput in-line stress-annealing technique within carefully controlled temperature and stress windows. However, stress annealing was only practical because of the high toughness of the Co60Fe20B15Nb5 alloy, which was maintained even after initial thermomechanical processing. Magnetic characterization, including B-H loop, core loss measurements, and magneto-optical-Kerr-effect (MOKE) microscopy, alongside mechanical fracture toughness screening, revealed that Co-based nanocrystalline soft-magnetic alloys can offer superior induced anisotropy and fracture toughness compared to Fe-based counterparts.

GS 15. Effect of Electropolishing on Morphology and Adhesion of Nanostructured Anodic Tantalum Oxide Thin Films

Presenter: Sarah Pooley, Boise State University

Cyrus Koroni, Boise State University
Shinthia Binte Eskender, Boise State University
Joshua Russell, Boise State University
Hui Xiong, Boise State University

Anodic tantalum oxide films have attracted significant interest for their highly favorable properties, such as corrosion resistance and biocompatibility, as well as the cost-effective and scalable nature of anodization as a fabrication method. However, the need for morphological control as well as strong adhesion of the resulting films to the substrate pose barriers to their application. In this work, the morphology and adhesion of anodic tantalum oxide films grown on electropolished, chemically etched, and pristine tantalum metal substrates in a fluoride-free electrolyte containing potassium phosphate and glycerol under varying voltage and temperature conditions were systematically investigated. Electropolishing significantly reduced substrate surface roughness and promoted the growth of native oxide/suboxide species. Current density-time characteristics during anodization suggest noticeable kinetic effects related to substrate pre-preparation, which were corroborated by significantly increased nanoporosity in oxide films grown on electropolished substrates. Systematic variation in voltage and temperature provided evidence of improved control over size and morphology of the nanoporous anodized oxide films via anodization parameters in electropolished samples. In addition, pull tests demonstrated increased film-substrate adhesion in anodized oxide films on both chemical etched and electropolished substrates. These findings demonstrate that electropolishing is an effective strategy for improving the controllability of nanostructure morphology, film uniformity, and adhesion of anodic tantalum oxide coatings.

GS 16. Understanding Microstructural Differences at Volumetric Energy Density Interfaces for Laser Powder Bed Fusion SS 316L

Presenter: Brandon King, Boise State University

Noah Montrose, Boise State University
Mike Hurley, Boise State University

Laser Powder Bed Fusion (LPBF) allows the creation of geometrically complex parts with material efficiency, more specifically with SS 316L. However, understanding and controlling the microstructure at the interfaces between zones printed with different Volumetric Energy Density (VED) parameters is an essential gap that requires addressing. While multiple VED printing is highly advantageous for print efficiency and residual stress control, the microstructural mismatch between the two zones can create mechanical and electrochemical complications. In order to better understand this interaction, four prints containing distinct regions of multi-VED interfaces were examined via SEM, EBSD, and electrochemical testing. XRD of the four prints and powder feedstock was also examined to verify phase composition. In addition, localized electrochemical testing was performed to determine differences in corrosion performance of the VED interfaces. The role of LPBF-induced sub-grain cellular structures on both dislocation movement and corrosion initiation was systematically analyzed. Additionally, electrochemical polarization of the printed matrix was explored as a method to produce surface nanostructures unique to LPBF stainless steel. These nanostructures potentially exhibit super hydrophobic and anti-biofouling properties, which are highly desirable for diverse industrial applications. By understanding the mechanisms that govern the formation of select microstructural features, the potential of LPBF technologies can be expanded from geometric complexity to tailored microstructural complexity.

GS 17. Elucidation of the Hematite Direct Reduction Mechanism Using In Situ Spectroscopy

Presenter: Casey Mezerkor, University of Oregon

Ravi K. Kukkadapu, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA, USA
Carinna L. Lapson, Department of Chemistry and Biochemistry and the Oregon Center for Electrochemistry, University of Oregon, Eugene, OR, USA/Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA, USA
Mark Bowden, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA, USA
Raj Shekhar, Department of Chemistry and Biochemistry and the Oregon Center for Electrochemistry, University of Oregon, Eugene, OR, USA
Eric D. Walter, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA, USA
Paul A. Kempler, Department of Chemistry and Biochemistry and the Oregon Center for Electrochemistry, University of Oregon, Eugene, OR, USA

J. David Bazak, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA, USA

Research on alternative energy storage technologies continues, especially in the grid-scale long duration space where traditional battery technologies (including lithium-ion) suffer from either cost or safety concerns. Conversion anodes leveraging multi-valent iron promise high capacities, but key microscopic details of the mechanism for conversion are unknown. Towards this objective, this study aims to use in situ electrochemical cells combined with NMR and EPR spectroscopy to search for reaction intermediates directly, expanding on previous studies where largely ex situ methods or carefully constructed surfaces and morphologies were employed. Performing the spectroscopic measurements under realistic electrochemical cell conditions which maximize the reaction conditions (strongly alkaline media, elevated temperatures > 60 C) and using synthetic hematite aggregates demonstrated i) a lack of dissolved Fe3+ and ii) the presence of solvated Fe2+ species which scaled with applied current density. Leveraging ex situ Mössbauer spectroscopy in combination with the in situ measurements yielded evidence for an initial reduction step of Fe3+ to Fe2+ within the hematite structure. Collectively, these findings point to a solid-state reduction mechanism for hematite via a maghemite intermediate, followed by rupture and dissolution/reduction, with the steady-state solvated Fe2+ concentration gradually dissipating after the applied potential is removed. Detailed mechanistic knowledge will help inform future efforts to engineer further improvements to the direct electrochemical iron oxide reduction process.

GS 18. Mechanistic Understanding of the Surface Modulation in Lead Acid Batteries

Presenter: Carinna Lapson, University of Oregon

D. Thien Nguyen, Pacific Northwest National Laboratory
Casey S. Mezerkor, University of Oregon
J. David Bazak, Pacific Northwest National Laboratory
Ajay S. Karakoti, Pacific Northwest National Laboratory

Further understanding on how various lignin additives impact lead negative active material in the presence of different H2SO4 concentrations provides new knowledge to the otherwise greatly studied lead acid battery system. When at lower concentrations (1 M), lignin expanders, such as calcium lignosulfonate (CaLS) and Vanisperse DCA, operate effectively by altering PbSO4 crystallization kinetics. Instead of forming an immediate and passive, compact layer of PbSO4 (seen in the no lignin control), even minimal lignosulfonate additions within the electrolyte open SO4- mass transport pathways to the underlying lead active material. When monitored in cyclic voltammetry experiments, CaLS exhibits the highest peak currents after 20 cycles, more than doubling the active surface area compared to the control. Conversely, at higher concentrations (5 M), the common ion effect suppresses Pb2+ solubility, driving instantaneous precipitation of PbSO4 and, when lignin variants are added, causes rapid volume expansion from Pb to which stresses the cohesion of the lignin-adsorbed surface to the bulk lead. Cyclic voltammetry experiments along with galvanostatic

cycling, static EIS with DRT analysis, SEM/EDS, and XPS studies expand initial experiments to provide additional insights on PbSO4 formation/dissolution behavior.

GS 19. Interfacial Structure and Metal Coordination in Crystalline Peptoid Membranes
Presenter: Wenhao Zhou, Pacific Northwest National Lab

The widespread structuring of water at interfaces and the coexistence of hydrophobic and hydrophilic regions in biological materials suggest that interfacial water plays a central role in molecular recognition, stability, and assembly. Inspired by this principle, we investigate the interfacial hydration structure of crystalline membranes formed by self-assembly of amphiphilic, sequence-defined biomimetic polymers known as peptoids, and examine how metal-ion coordination modulates their structure and hydration. Using highly ordered pyrolytic graphite (HOPG) as a model hydrophobic substrate, high-resolution atomic force microscopy (HR-AFM) was used to resolve membrane assembly, molecular packing, and lattice order, while three-dimensional AFM (3D-AFM) probed interfacial hydration and local mechanical response. Peptoids assemble into monolayer-thick membranes consisting of molecular rows with long-range crystalline order and exhibit well-defined hydration structures that reflect the underlying membrane lattice. Comparison of metal-free membranes with those coordinated by divalent metal ions, including Zn^{2+} and Co^{2+}, reveals that metal ions bind within domains aligned with the peptoid rows and coordinate adjacent rows, doubling the lattice parameter perpendicular to the row direction. 3D-AFM further reveals distinct hydration signatures associated with metal-peptoid coordination, manifested as changes in force-gradient profiles and interfacial contrast without disrupting crystalline order. These results establish connections among sequence-defined peptoid chemistry, metal-ion coordination, and interfacial hydration in hierarchical membrane architectures, and demonstrate the potential of crystalline peptoid membranes as bioinspired templates for controlled multilayer growth and mineralization toward architected soft materials with programmable structure and multifunctionality.

GS 20. Fundamental Study and System Development of Radical-mediated Electrochemical Reactions for Biogas Upgrading
Presenter: Yongjun Kwon, Washington State University

Qiaowan Chang, : Washington State University
Binhong Wu, : Washington State University
Liyue Zhang, : Washington State University

Two key greenhouse gases, methane (CH4) and carbon dioxide (CO2), can be mitigated by valorizing biogas streams via upcycling into higher-value chemical products. Traditional upcycling relies on high-temperature thermochemical reforming; however, the strong C–H and C=O bonds in these molecules impose a high activation energy barrier, requiring extreme operating temperatures (700–900 °C) whose energy demands hinder commercial deployment. To bypass these thermal barriers, we demonstrate an electrochemical radical-mediated system capable of converting biogas under

mild conditions. By generating reactive radical species, this approach overcomes traditional activation limits to enable simultaneous, room-temperature conversion of both CH4 and CO2. Specifically, using a dual-cathode H-cell system, an oxidized carbon nanotube (OCNT) cathode generates a controlled flux of H2O2, which then undergoes Fenton-like cleavage at a secondary iron oxyfluoride (FeOF) cathode, thereby driving conversion. Furthermore, we optimized gas mixture ratios to evaluate feed dynamics and radical utilization systematically. The system exhibited a maximum total product production of 3.811 umol at a 5:1 CH4:CO2 ratio, yielding formic acid, methanol, methyl hydroperoxide, and acetic acid. To resolve key mechanistic ambiguities regarding CO2 activation, spin-trapping experiments using 5,5-dimethyl-1-pyrroline N-oxide (DMPO) isolate the initiating agent—differentiating between hydrated electron attack and hydrogen radical intermediates, identifying the hydrated electron as the dominant activating species for CO2. By deciphering interfacial radical–reactant interactions, this research establishes a way to bypass these thermal limitations, enabling efficient, single-step biogas upcycling under mild conditions.

GS 21. Enhancing Metal-Free Carbonic Anhydrase Mimics via Active-Site Residue Modification with Peptoid Nanosheet Co-Assembly

Presenter: Sebastian Peck, Pacific Northwest National Lab

Thi Kim Hoang Trinh, : Pacific Northwest National Lab
Chun-Long Chen, : Pacific Northwest National Lab, University of Washington

Carbonic Anhydrase (CA), an enzyme present in nearly every living organism in one form or another, excels at the conversion of CO2 into the more biologically useful HCO3-. Across the eight known species of CA, this conversion mechanism is primarily driven by the interplay of a central metallic active site in all but one species, and the geometry and effects of surrounding amino acid residues. CA's ability is sought after for carbon capture, agriculture, and greener fuel production, but direct use is limited by its synthesis complexity and lack of stability. Synthetic CA mimics help bridge this gap - rather than creating novel enzymes from long protein sequences, these mimics instead use self-assembled macromolecules to create active-site analogues. To reduce the resources needed for these catalysts, researchers have developed CA mimics that forgo the metallic ion cofactor altogether, relying instead on amino acids like groups of histidine working in conjunction to enable the proton transfer mechanism for hydration. Poly-N-Substituted-Glycines (Peptoids) are an achiral cousin to peptides that enable more control over self-assembled structures, allowing for multifunctional and multi-domain 2-D nanosheets. Peptoid nanostructures have been proven to be effective as metal-containing CA mimics, but by leveraging their ability to create macroscopic structures and multifunctional domains, it becomes possible to also make them into effective metal-free mimics. By co-assembling peptoids with Histidine, Cysteine, and Glutamate residues, we demonstrate their ability to self-assemble into nanosheets, as well as their performance in 4-NPA hydrolysis and direct CO2 mineralization.

Undergraduate Students Posters

UGS1. Understanding Growth and Evolution of Tungsten Oxide Thin-Films Via Programmable Chemical Vapor Reactor

Presenter: Anton Escher, Oregon State University

Anton Escher , School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR 97331
Kylee Lamberson, School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR 97331
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Most common direct writing techniques such as Inkjet printing, Aerosoljet printing and material extrusion use solvent based inks which leave residual impurities. Chemical Vapor deposition (CVD) is the most widely used thin-film deposition technique which eliminates these issues. However, CVD uses deposition chambers where substrates are fed into. Although prior works show scanning nozzle deposition, they fall short in showing how moving nozzle and substrate affect the growth mechanism and morphology. In this work, a modular chemical printer enabled by micro-reactor assisted nanomaterial deposition (MAND) will be presented. We will discuss the modular reactor's capability of dry printing patterned thin films by studying the growth mechanism and morphological evolution using Atomic Force Microscopy (AFM), scanning electron microscopy (SEM), and X-ray diffraction (XRD). Furthermore, we tested the capacitance of the tungsten oxide thin films grown on FTO and silicon substrates. We found that our films showed capabilities for energy storage, by showing between 4 mF.cm^-2 and 15 mF.cm^-2 areal capacitances.

UGS 2. Calculating the stability of layered oxysulfide perovskites for solar energy conversion

Presenter: Elizabeth Sterley, Western Washington University

Lucas Ramsdale, Department of Chemistry, Western Washington University
Robert F. Berger, Department of Chemistry, Western Washington University

Semiconductors crystallizing in the perovskite structure have been studied for a variety of applications, including solar energy conversion. While halide perovskites for photovoltaic solar cells have received more attention in the past decade, oxide perovskites show promise as water-splitting photocatalysts. Transition metal oxides like SrTiO3, however, are limited in their ability to absorb sunlight due to their relatively large band gaps. Fully or partially substituting other chalcogenide anions (S, Se, Te) for oxide could potentially lower these band gaps, though only a few chalcogenide or oxychalcogenide perovskites exist - presumably due to the larger size of sulfide, selenide, and telluride anions. In this work, we use density functional theory (DFT) to computationally assess the energetic stability and synthetic viability of novel oxychalcogenide perovskites whose geometric environments are designed to stabilize larger anions. Inspired by the existence of a small number of oxysulfide compounds like Y2Ti2O5S2 that resemble layered perovskites, we focus on Ruddlesden-Popper phases with the general formula A2BO2X2. We use DFT to 1) compare their energies to a variety of competing binary and ternary structures, and 2) compute the thermodynamics of using gas-phase reagents like CS2, H2S, H2Se, and H2Te to incorporate chalcogenide anions into oxide compounds. In doing so, we identify several promising compounds and also show that our predictions are consistent with traditional arguments for stability based on ionic radii.

UGS 3. Synthesis of Silver Nanostructures on Silk Fibroin Microparticles via Direct Seed Mediated Growth

Presenter: Ava Kimel, Western Washington University

Nikki Nikolas, Western Washington University
Ying Bao, Western Washington University
Amanda Murphy, Western Washington University

The combination of biopolymer silk fibroin with plasmonic metal nanoparticles can be used to create unique composite materials for a variety of applications including surface enhanced Raman spectroscopy (SERS). This study investigates the direct growth of silver nanostructures on chemically modified silk microparticles using a seed-mediated approach. The effects of using a seed-mediated approach, reaction kinetics, and varying growth solution parameters were explored. The resulting composites were characterized using SEM, with the goal of testing their sensing performance using surface enhanced Raman scattering (SERS).

UGS 4. Precipitation and Modification of Silk Fibroin Particles to Interface with Metal Plasmon Resonators

Presenter: Nikki Nikolas, Western Washington University

Ava Kimel, Megan Downer, Camden Losey, Annabella Talbot, Prof. Ying Bao, Prof. Amanda Murphy, Department of Chemistry, Western Washington University, Bellingham, WA

Strategies for integrating the biopolymer silk fibroin with metal nanomaterials are explored to create flexible, biocompatible substrates for sensing applications. Silk fibroin is a naturally derived, biodegradable material with excellent mechanical strength and widespread use in biomedical settings. In this work, the silk surface and gold seed ligand were chemically modified to enable electrostatic attachment and/or growth of metal nanostructures on silk microparticles. The resulting composites were characterized using SEM, DLS, and zeta potential with the goal of testing their sensing performance using surface enhanced Raman scattering (SERS).

High School Students Posters

HS1. PNNL High School Summer Research Internship in Critical Materials Recovery

Presenter: Sanah Khan, Pacific Northwest National Lab

During the summer of 2026, I completed a High School Research Internship (HSRI) at Pacific Northwest National Laboratory (PNNL). I worked with the Nucleation & Growth Team on recovering valuable materials from spent batteries and samarium-cobalt (SmCo) magnets. Through this experience, I developed hands-on laboratory skills by preparing ammonium sulfate and sulfuric acid stock solutions, preparing and diluting leachate samples for Inductively Coupled Plasma Mass Spectrometry (ICP-MS) analysis, monitoring and adjusting pH, performing electrochemical leaching experiments, and collecting and documenting experimental data. I also prepared solid residues using X-ray diffraction (XRD) to evaluate the effectiveness of the leaching process. Additionally, I gained experience using SolidWorks and 3D printing to design and create laboratory components. Working in a research environment strengthened my laboratory skills and increased my confidence in conducting scientific research. This experience also deepened my interest in chemistry, materials science, and research. I learned the importance of teamwork, problem-solving, and communication for solving real-world challenges in sustainable materials research.

General Posters

PS 1. **Surface Engineering of Beta-Alumina Solid Electrolytes with Salt-Modified Sodiophilic Porous Carbon for Molten-Sodium Batteries**

Presenter: Henry Han, Pacific Northwest National Laboratory

J Mark Weller, Pacific Northwest National Laboratory
Joseph P Quinn, Pacific Northwest National Laboratory
David M Reed, Pacific Northwest National Laboratory
Guosheng Li, Pacific Northwest National Laboratory

The interfacial behavior between molten sodium and beta-alumina solid electrolyte (β''-Al2O3, BASE) critically determines the electrochemical performance and operating temperature of molten-sodium batteries. However, intrinsically poor sodium wettability on BASE causes non-uniform physical contact, limited interfacial charge transfer, and high polarization, particularly below 200 °C. Here, we present a scalable, cost-effective, and metal-free strategy for modifying BASE with a self-functionalized sodiophilic meso/microporous carbon layer. The coating is fabricated by spray coating an aqueous mixture containing a nonionic Tergitol surfactant, hydroxypropyl methylcellulose (HPMC) as a water-soluble binder, carbon, and selected sodium salt additives, followed by annealing at 350 °C in air. The binder-controlled porous structure provides interconnected channels that promote capillary infiltration and lateral transport of molten sodium across the BASE surface. Meanwhile, the sodium salt additives modify the surface characteristics of the carbon layer, enhance its affinity toward molten sodium, and strengthen its adhesion and mechanical stability on the ceramic substrate. The combined effects of surface chemistry and hierarchical porosity produce more uniform Na/BASE interfacial contact, reduce polarization and cell overpotential, and improve the electrochemical performance of Na/BASE/Na symmetric cells at operating temperatures of 110°C–190°C. In particular, phosphate-based salt additives provide a substantial improvement in sodium wettability and interfacial stability. These results demonstrate how controlling surface composition, pore structure, and interfacial interactions can enable effective wetting of solid electrolytes without conventional metal-based coatings. This surface-engineering strategy provides a practical route toward durable, low-resistance interfaces for lower-temperature molten-sodium batteries.

PS 2. **Optical Bandgap Engineering and Magnetic Responses in Hybrid Halide Frameworks**

Presenter: Khyati Anand, Pacific Northwest National Lab

Kavin Chakravarthy Thangaraj, : Pacific Northwest National Lab, Rachel Rasbach, : California State University San Bernardino, San Bernardino

Skye Blanks, : California State University San Bernardino, San Bernardino
Kirill Kovnir, : Ames National Laboratory, Division of Materials Science and Engineering
Genevieve Amobi4, : Department of Chemistry, Iowa State University, Ames, Iowa 50011, USA
Joyce Pham, : Department of Chemistry, California State University San Bernardino, San Bernardino, CA, 92407, US
Shannon Lee, : Pacific Northwest National Lab

Hybrid organic–inorganic halide materials offer a versatile platform for investigating the interplay between crystal structure, optical response, and magnetism. In this work, the structural, optical, and magnetic properties of a family of related halide compounds were examined. Diffuse-reflectance measurements revealed a pronounced decrease in reflectance in the ultraviolet region below approximately 300 nm, consistent with strong ligand-to-metal charge-transfer transitions and absorption associated with the halide lattice. Kubelka–Munk analysis and Tauc plots were used to estimate the optical band gaps, with the direct-transition model providing the most reliable linear behavior near the absorption edge. Magnetic susceptibility measurements reveal predominantly paramagnetic behavior at elevated temperatures, with low-temperature magnetic anomalies occurring in the approximate range of 5–10 K. Curie–Weiss analysis was used to evaluate the effective magnetic moments and magnetic exchange interactions. In contrast, field-dependent magnetization measurements at low temperature demonstrate composition-dependent responses and approach saturation at high applied fields. These results highlight how structural dimensionality and cation-induced changes in the metal–halide framework influence the magnetic and optical properties of hybrid manganese halides, providing useful guidelines for the design of new molecular–inorganic materials.---

PS 3. Atomic-scale insights into antiphase boundaries in Fe3O4 and high-entropy spinel thin films
Presenter: Ding Peng, Pacific Northwest National Lab

Antiphase boundaries (APBs) are well known defects that affect the optical and electronic performance of ordered oxides. Yet resolving APBs in three dimensions—particularly along the beam direction—remains a significant challenge. Depth-sectioning STEM suffers from limited axial resolution due to geometric and chromatic aberrations, while strong electron-channeling in crystalline materials further complicates contrast interpretation. In this work, we demonstrate that depth-sectioning HAADF-STEM, combined with comprehensive multislice simulations, enables direct visualization of the three-dimensional structure of APBs. Epitaxial Fe3O4 and high-entropy spinel oxide thin film grown by molecular beam epitaxy (MBE) serves as ideal platforms, as controlled variations in growth temperature, cation-flux stoichiometry, and oxygen pressure naturally generate a wide range of APB morphologies. By acquiring a focal series and reconstructing depth-dependent contrast, we map the spatial distribution of APB-induced domains and reveal complex networks where multiple boundaries intersect at distinct crystallographic orientations. Interpretation of the antiphase translation vector is carried out through a semi-quantitative multislice-based pattern-matching approach, which requires prior knowledge of specimen thickness and geometry.

This strategy is conceptually related to quantitative STEM efforts such as those by Van Aert and co-workers, but here it is applied in a semi-quantitative manner using multislice simulations to capture strong channeling in a non-thin specimen, enabling identification of the APB configurations most consistent with the observed contrast. Rather than relying on depth-sectioning alone, the strength of this method lies in the multislice-guided interpretation of the focal-series STEM contrast, which enables robust determination of APB configurations in three dimensions.

PS 4. **Crystallization Induced H/D Exchange in Water Examined From 141 to 149 K**
Presenter: Amal Berhan, Pacific Northwest National Lab

Loni, Kringle, Pacific Northwest National Lab
Megan , Dunlap, Pacific Northwest National Lab
Scott, Smith, Pacific Northwest National Lab
Greg , Kimmel, Pacific Northwest National Lab

Autoionization of water, or the formation of hydronium (H3O+) and hydroxide (OH-) ions, is a fundamental process in chemistry. The rarity and rapid timescale of water disassociation has limited our understanding of autoionization and its associated dynamics, particularly at cryogenic conditions. Here, we examine proton (H/D) exchange using layered H2O and D2O nanoscale films at temperatures between 141 and 149 K as an indicator of the autoionization process – by suppressing the exogenous sources of protons,1 the protonated species involved in the exchange reaction is surely a result of autoionization within the film. We use reflection absorption infrared spectroscopy to track the formation of HOD molecules due to H/D exchange. While we do not observe significant HOD formation within the liquid configuration, there is, however, significant H/D exchange occurring with the onset of crystallization. We therefore hypothesize the autoionization of water was driven by crystallization induced dipolar ordering. We also find that the relative magnitude of H/D exchange decreases with increasing temperature and increasing concentration of D2O molecules within the film. 1 Smith, et al., J. Chem. Phys. 149, 081104 (2018).

PS 5. **Interfacial control of framework growth and critical-mineral recovery**
Presenter: Sun Hae Ra, Pacific Northwest National Laboratory

Controlling reactions at solid-liquid and electrode-solution interfaces is essential for designing functional materials. Here, we present two applications of interfacial chemistry: crystallographic control of two-dimensional conductive metal-organic framework (2D c-MOF) films and selective recovery of rare-earth elements (REEs) using polyoxometalate (POM)-based adsorbents. During anodic electrodeposition of 2D c-MOF, the applied potential regulates interfacial linker oxidation and nucleation. Deposition at lower potential favors pronounced (002) texture, consistent with layers predominantly parallel to the substrate, whereas increasing potential suppresses the (002) contribution and increases the relative prominence of low-angle associated with the (100) family indicating a shift in preferred orientation toward (100). At the solid-liquid interface, the oxo-rich

phosphotungstate cluster provides a molecular recognition platform for REE capture from saline waters. Water-insoluble POM adsorbents exhibit selective REE uptake over abundant competing ions. Polymer incorporation further modifies the local coordination environment, enhancing adsorption and improving desorption and regeneration. Together, these studies demonstrate how interfacial control and surface characterization enable functional materials for oriented coatings and critical-mineral separations.

PS 6. Optimization pH Stability Mapping and Automated Data Management in All-Iron Redox Flow Battery Electrolyte Screening

Presenter: Sophie Liu, Pacific Northwest National Laboratory

We present a data-driven framework for optimizing all-iron redox flow battery electrolytes, coupling a custom PostgreSQL relational database (optpH) with Bayesian optimization (BO) to accelerate additive discovery for improved ferric ion pH stability. Experimental data are automatically uploaded to the database, which comprises six table types centered on the result_run (per-sample formulation data, pH, and visual clarity) and summary_run tables, supported by lookup libraries, metadata, and a data dictionary to ensure long-term reusability. Using this structured dataset, BO modeled and optimized pH and visual clarity across three models, with curated inputs excluding non-equilibrium and unreliable data points. The framework identified new formulation candidates for high-throughput assessment.

PS 7. Fabrication of Foam Targets for Laser Produced Plasma Based EUV Generation

Presenter: Peipei Wang, Pacific Northwest National Laboratory

Ray Tyler , Pacific Northwest National Laboratory
Matthew Polek, Pacific Northwest National Laboratory
Hari Harilal, Pacific Northwest National Laboratory
Ajay Karakoti, Pacific Northwest National Laboratory

Extreme ultraviolet (EUV) lithography at 13.5 nm is the enabling technology for advanced semiconductor manufacturing, where higher source efficiency, improved spectral purity, and reduced debris generation are critical for next-generation EUV light sources. Low-density, mass-limited metal targets have emerged as a promising approach to overcome the limitations of conventional bulk Sn targets by reducing plasma opacity, suppressing debris formation, and improving in-band EUV emission. However, synthesizing porous foams with controlled density, tailored morphology, and homogeneous metal distribution remains a significant challenge. This work investigates the fabrication and characterization of low-density metal-doped porous foams as laser-produced plasma (LPP) targets. Two low-Z foam platforms were evaluated: conventional resorcinol-formaldehyde (RF) aerogels and bio-derived nanocrystalline cellulose (CNC) foams. Both platforms were doped with high-Z metals, including Sn for 13.5 nm EUV generation and Gd for 6.7 nm emission, to assess their suitability as mass-limited LPP targets. The materials were systematically

compared in terms of synthesis reproducibility, morphology, surface area, pore structure, and metal dispersion using complementary in-situ and ex-situ characterization techniques. These structural properties were then correlated with EUV emission characteristics to evaluate the influence of foam architecture on plasma behavior and spectral performance. The results demonstrate the advantages and limitations of RF and CNC foam platforms for producing uniform, low-density metal-doped targets. This study provides insights into the design of optimized porous target materials that enable cleaner, more efficient laser-produced plasma sources for next-generation EUV lithography and related short-wavelength photon applications.

PS 8. Resolving Surface Chemistry at Soil Mineral - Organic Interfaces Across MONet Soils: A High-Throughput Multimodal Approach

Presenter: Kavin Thangaraj, Pacific Northwest National Laboratory

Vaithiyalingam Shutthanandan , Pacific Northwest National Laboratory
Catherine Jane Pettinger, University of Wisconsin
Mark Enelhard, Pacific Northwest National Laboratory
Odeta Oafoku, Pacific Northwest National Laboratory
Bhuvaneswari Modachur Sivakumar, Pacific Northwest National Laboratory
Ravi Kumar Kukkadapu, Pacific Northwest National Laboratory
Ajay Karakoti, Pacific Northwest National Laboratory

Resolving how soil carbon becomes stabilized as mineral-associated organic matter (MAOM) at the molecular scale is a prerequisite for representing soil processes accurately in Earth system models. Much of that picture rests on the chemistry and spatial organization of organic matter (OM) at mineral interfaces, including the mechanisms by which ions bind, the distribution and density of reactive sites, and the arrangement of functional groups. These properties govern the persistence, transformation, and loss of soil carbon. To address these questions, we developed a high-throughput multimodal imaging and spectroscopy workflow that describes mineral-organic interfaces in terms of elemental composition, molecular structure, and micro- to nanoscale topology. The workflow combines X-ray photoelectron spectroscopy (XPS), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS), which together report on bonding environments, functional group chemistry, surface morphology, and mineral composition. Data collection is supported by a custom high-throughput sample preparation method that allows multiple soil blots or mineral-OM extracts to be prepared rapidly and reproducibly on a single substrate. Because all four techniques then probe a comparable region of the sample, chemical and structural measurements are directly comparable across methods. The platform handles approximately 50 samples per day, which makes systematic characterization of MAOM across environmental gradients practical at scale. Samples for this study were drawn from the MONet project, a broad and spatially diverse soil inventory suited to establishing quantitative

relationships between mineral surface properties, organic matter chemistry, and carbon stabilization.