AVS Prairie Chapter Symposium on Materials Research Topics

August 7, 2025

Lake Forest College
Lake Forest, IL 60045, USA

Schedule/Abstract Book

Conference Organization

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Special Acknowledgments

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Welcome

Dear Participants,

It is our great pleasure to welcome you to the AVS Prairie-Chapter Symposium at Lake Forest College. This special gathering brings together researchers and students from across the Midwest to share their latest findings and innovations. This year's program features over 45 presentations across multiple tracks, including keynote speeches from distinguished scientists, technical sessions, and poster presentations. We have carefully curated a diverse program that represents the breadth and depth of current research trends and technologies. We hope that the meeting will inspire new collaborations in our regional materials-science community and contribute to the advancement of knowledge in your respective fields.

The symposium is hosted on the scenic Lake Forest College campus, whose architectural charm and peaceful atmosphere lend a unique character to our gathering. We invite you to take time during your visit to explore the campus grounds and to stop by our holography gallery at the Lillard Science Center after the symposium.

We offer our heartfelt gratitude to our sponsors: Alan Burrill Technical Sales, AVS, Midwest Vacuum, Scroll Labs, Vacuum One, VAT. Their generous support made this conference possible. We also extend sincere thanks to our program committee members, whose work was essential in ensuring the high standard of our technical program. A special thanks goes to the faculty and staff at Lake Forest College. Your assistance in planning and organizing the event has been invaluable.

Welcome once again, and we wish you a productive and enjoyable meeting experience. Please do not hesitate to reach out to our organizing committee members if you need any assistance during the event.

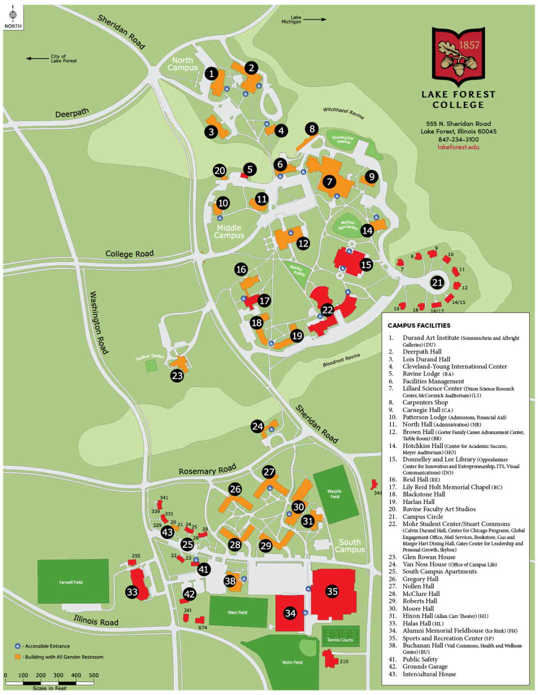
2025 AVS Prairie Chapter Symposium program committee

Venue

The AVS Prairie Chapter 2024 Symposium will be held on the campus of Lake Forest College in the Tarble Room of Brown Hall shown below. Brown Hall is building number 12 on the campus map.

Brown Hall

Campus map



Parking

Free parking is available on campus for symposium participants near Brown Hall and surrounding buildings. No special parking permit is required. Stay away from spots marked with a red sign, as they are designated for specific purposes.

Wi-Fi

Use the Wi-Fi network: ForesterGuest

Schedule

8:00-8:30	Registration
8:30-8:40	Welcome Remarks
	SESSION A
8:40-9:30	INVITED TALK: **Elijah Thimsen**, *Washington University at St. Louis*, "Nonequilibrium Plasma for Synthesis and Stabilization of Materials Under Extreme Chemical Potential of Conjugate Gas"
9:30-9:45	**Feray Buyuktopcu**, *University of Illinois Urbana-Champaign*, "Tandem Plasma and Electrochemical Treatment for Near-Complete Defluorination of PFOA"
9:45-10:00	**Nathaniel McNeilly**, *Michigan State University*, "Mem-Energy: A Detailed Energy Estimation for Membrane Processes Undergoing Fouling"
10:00-10:15	**Isaiah A. Adams**, *Northwestern University*, "Probing the Growth Mechanisms of ALD on Chemically "Inert" Polymers"
10:15-10:35	Coffee Break & Poster Presentations (20 min)
	SESSION B
10:35-10:40	**Outstanding Research Award Presentation** (5 min)
10:40-11:30	2025 AWARD TALK: **Matthew Gebbie**, *University of Wisconsin-Madison*, "Linking Electric Double Layer Formation to Electrocatalytic Activity "
11:30-11:45	**Nileema Sharma**, *University of Notre Dame*, "Atomic-scale Frustrated Josephson Coupling and Multi-condensate Visualization in FeSe"
11:45-12:00	**Vinod K. Sangwan**, *Northwestern University*, "Video-Rate Infrared Camera Based on Solution-Processed Black Phosphorus Films "
12:00-12:50	Lunch Break (50 min)
12:50-1:30	Poster Presentations (40 min)
	SESSION C
1:30-2:20	INVITED TALK: **Arashdeep Thind**, *University of Illinois at Chicago*, "Exploring materials atom-by-atom using electron microscopy"
2:20-2:35	**Ayoyele Ologun**, *University of Illinois at Chicago*, "Surface Properties of Zirconium Diboride (0001) and Homoepitaxial Growth of Zirconium Diboride as Determined by Scanning Tunneling Microscopy"
2:35-2:40	**Outstanding Research Award Presentation** (5 min)
2:40-3:30	2024 AWARD TALK: **Teri W. Odom**, *Northwestern University*, "Designer Material Metasurfaces"
3:30-3:45	**Alexis Gonzalez**, *Loyola University Chicago*, "Oxygen Diffusion Dynamics on a Rh (111)/(322) Bifaceted Surface"
3:45-4:05	Coffee break & Poster Presentations (20 min)
	SESSION D
4:05-4:55	INVITED TALK: **Hakim Iddir**, *Argonne National Laboratory*, "Insights from Atomistic Modeling of Battery Materials"
4:55-5:10	**Maxwell Gillum**, *Loyola University Chicago*, "Steps Accelerate the Formation of Rhodium Surface Oxide"
5:10-5:25	**Jorit Obenlueneschloss**, *Ruhr University Bochum*, "Electrocatalytic-HER Active RuS_2 Thin Films from a New CVD Process"
5:25-5:40	**Jessica Jones**, *Argonne National Laboratory*, "Electric Field-Modulated Atomic Layer Deposition for Modification of Thin Film Properties"
5:45-6:45	**Awards Ceremony and Closing**

Plenary Talks

Nonequilibrium Plasma for Synthesis and Stabilization of Materials Under Extreme Chemical Potential of Conjugate Gas

Elijah Thimsen*

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Nonequilibrium plasma can synthesize and stabilize materials that contain elements that form conjugate gases, such as nitrogen, at temperatures and partial pressures where those materials would otherwise be unstable without the plasma.[1] For example N_2, the conjugate gas of nitrogen in GaN, is released at high temperatures and low N_2 pressures without plasma.[2, 3] Historically, the reactivity of the plasma has been understood by the concept of a "dominant species", where the idea is that one type of species such as atomic N, or vibrationally-excited $N_2(\nu)$, or electronically excited N_2(A), is *the* important reactive species.[4, 5] However, experimental evidence for the idea of a dominant species is often ambiguous, or altogether absent, since the density of multiple excited species are correlated, such as N and $N_2(\nu)$ increasing together[4] with process parameters. To address the situation where multiple excited states may contribute to the reactivity of a nonequilibrium plasma, our goal has been to advance a new way to quantify the reactivity at the population level that does not require a dominant species. This new concept of plasma activation describes the reactivity of the plasma as an additional chemical potential that an ideal conjugate gas would need for the material (e.g. metal-nitride) to react in the same way as it does to the plasma. The additional chemical potential is thought to depend on the plasma, not the material that the plasma is in contact with. This concept will be illustrated using examples of temperature stability of indium nitride and gallium nitride at low N_2 partial pressures where these materials are thermodynamically and kinetically unstable in the absence of the plasma. Use of the concept for assessing the feasibility of proposed material synthesis processes will then be described.

References

1. Moher, D., R. Shanahan, and E. Thimsen, Stabilization of III-nitrides at high temperatures using nitrogen plasma. Applied Physics Letters, 2025. **126**(15): p. 151903.
2. Karpiński, J., J. Jun, and S. Porowski, Equilibrium pressure of N_2 over GaN and high pressure solution growth of GaN. Journal of Crystal Growth, 1984. **66**(1): p. 1-10.
3. Karpiński, J. and S. Porowski, High pressure thermodynamics of GaN. Journal of Crystal Growth, 1984. **66**(1): p. 11-20.
4. Bayer, B.N., P.J. Bruggeman, and A. Bhan, Species, Pathways, and Timescales for NH_3 Formation by Low-Temperature Atmospheric Pressure Plasma Catalysis. ACS Catalysis, 2023. **13**(4): p. 2619-2630.
5. Bayer, B.N., et al., Availability and reactivity of $N_2(\nu)$ for NH_3 synthesis by plasma catalysis. Plasma Sources Science and Technology, 2023. **32**(12): p. 125005.

Designer Material Metasurfaces

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Optical metasurfaces are engineered planar structures with rationally designed building blocks that can manipulate light in new ways. However, less attention has been devoted to surface chemistry, materials, and interfaces of the units or their integration with responsive materials. This talk will discuss current advances and prospects in manipulating light at the nanoscale using plasmonic nanoparticle lattices. These meta-materials support collective hybrid resonances with both light scattering and localized properties. First, we will describe the expanded scope of plasmonic lattices based on exquisite tuning of topological symmetries and surface engineering of the nanoparticles. Next, we will highlight how the nanoscale cavities combined with colloidal quantum emitters show unprecedented nano-lasing properties and strong coupling effects. Finally, we will discuss how this platform is opening diverse sensing opportunities from auto-regulatory materials to controlling cellular responses to long-range remote detection at room temperature.

Linking Electric Double Layer Formation to Electrocatalytic Activity

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Electrochemical reaction rates and selectivity often hinge on processes occurring at charged electrode-electrolyte interfaces, where molecular forces cause electrolyte ions to be attracted to or repelled from interfacial environments. Generally, oppositely charged counterions are attracted to and like-charged co-ions are repelled from interfaces, leading to charge separation that screens surfaces. Yet, this ion demixing incurs substantial entropic penalties. While double layer formation has remained an active area of research for more than a century, most frameworks used to predict electric double layer properties remain rooted in classical theory, which neglects ion-ion interactions. Yet, studies increasingly reveal that ion-ion interactions fundamentally alter double layer formation and interface properties. I will present our work aimed at linking ion assembly at ionic liquid-solid interfaces to the rates and selectivity of CO_2 reduction as a model system for illuminating how collective ionic assembly influences electrocatalytic activity. I will also discuss our discovery that co-ions can play a defining role in electrocatalytic reactions under the high surface potentials that are ubiquitous in electrochemistry, even under conditions where the bulk electrolyte is expected to behave classically. I will conclude with our perspective on how bridging advances from the colloid science and electrocatalysis fields opens the door to using reaction rates and selectivity as powerful tools to study electric double layer formation in concentrated electrolytes to open new frontiers in modulating reactivity at solid-liquid interfaces.

Exploring materials atom-by-atom using electron microscopy

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To develop a fundamental understanding of the materials around us, it is imperative to investigate structure-property relationships at the atomic-scale. A scanning transmission electron microscope (STEM) is a versatile tool that allows for the atomic-scale characterization of structure, chemical identity, and bonding environments for a variety of materials. STEM utilizes numerous analytical detectors that enable simultaneous imaging and spectroscopy experiments, which reveal a comprehensive view of the atomic-scale world. In this talk, using STEM experiments, I will reveal the interplay between structure and functionalities for a wide variety of material systems, including semiconductors, nanoplasmonics, battery cathodes, superconductors, and wide-gap oxides. For semiconductors and battery cathodes, I will show how atomic-scale defects and chemical heterogeneities impact the device performance. In phosphide-based nanoplasmonics, the interplay between vacancy formation, morphology, and plasmonic response will be established using atomic-scale STEM experiments and theoretical calculations. I will examine the layer-by-layer evolution of defect formation in Ruddlesden-Popper and infinite-layer nickelates, which has implications for high-temperature superconductivity. In a dielectric gate oxide, I will investigate the effect of high compressive strain during growth on its phase stability, octahedral tilts, and structural/chemical heterogeneities. Additionally, I will discuss some of the exciting recent developments in electron microscopy, including direct electron detectors, monochromatic electron sources, and magnetic-field-free pole pieces. The atomic-scale insights gained from electron microscopy can be transformative for materials research and, hence, can accelerate the realization of new functionalities for a diverse set of materials.

Insights from atomistic modeling of battery materials

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Cathode materials with improved energy densities, longer cycle-life, and improved safety characteristics are needed for portable electronic devices, smart grid systems, and transportation technologies. The highest energy-density cathode materials are based on transition metal oxides, such as layered $LiMO_2$ (M= Co, Ni, Mn), and and lithium and manganese-rich composite layered transition metal oxide (LMR-NMC) materials. These cathode materials can address some of the challenges associated with next-generation energy storage devices. However, sufficient knowledge on the atomic scale structure, local environment, and processes governing these metrics in working cells is still lacking. Herein, I will present few examples of current interest to the Li-ion battery research community using density functional theory and molecular dynamics to provide few insights on select structure-property relationships, elemental segregation, surface reconstruction, cathode-electrolyte interaction, bulk stability, and Li transport.

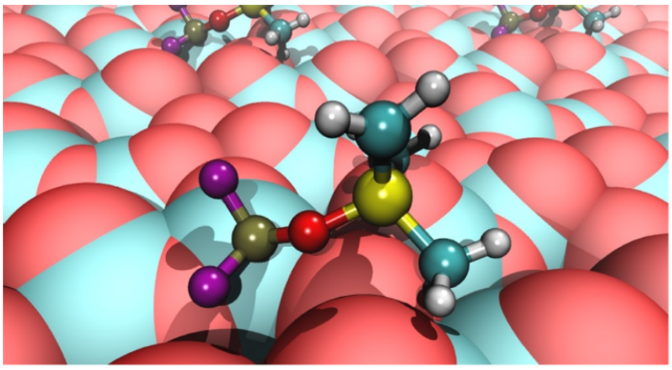

Figure 1: Surface models to investigate: Surface reconstructions, elemental composition-segregation, surface-electrolyte interaction, and metal dissolution. Image taken from: Chemical "Pickling" of phosphite additives mitigates impedance rise in Li ion batteries. Cameron Peebles, Juan Garcia, Adam P. Tornheim, Ritu Sahore, Javier Bareno, Chen Liao, Ilya A. Shkrob, Hakim H. Iddir, Daniel P. Abraham. The Journal of Physical Chemistry C 122(18), 2018.

Contributed Talks

Oxygen Diffusion Dynamics on a Rh (111)/(322) Bifaceted surface

Alexis Gonzalez[1], Elizabeth Serna-Sanchez[1], Maxwell Gillum[1], Stephanie Danahey[1], Johannes Diedrich[2]

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Understanding how surface structure influences oxidation processes is essential for advancing the design of metal-based catalysts. In this study, we investigate oxygen adsorption and diffusion on a bifaceted Rh (111)/ (322) single crystal using low-energy electron diffraction (LEED) and temperature-programmed desorption (TPD). The (111) facet represents a flat, close-packed surface, while the (322) facet introduces stepped features with more undercoordinated atoms. Our results reveal pronounced structure sensitivity: at 600 K, both facets form surface oxides, but LEED shows sharper oxide splitting on Rh (322), indicating more extensive oxide formation on the highly stepped surface. Notably, the Rh(322) facet also forms oxide at 350 K, where Rh(111) does not, underscoring the enhanced reactivity of step sites. At cryogenic temperatures, atomic oxygen exposures lead to high coverage on both facets; however, LEED reveals an ordered overlayer on Rh(111) and a faint ordered overlayer on Rh (322). Despite similar oxygen binding energies inferred from TPD, the structural response differs significantly with surface geometry. These findings highlight the critical role of facet-specific coordination environments in dictating oxidation behavior and providing insights into oxygen mobility across catalytic surfaces.

Atomic-scale Frustrated Josephson Coupling and Multi-condensate Visualization in FeSe

Nileema Sharma[1], Matthew Toole[1], James McKenzie[1], Sheng Ran[2], Xiaolong Liu[1]*

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In a Josephson junction involving multi-band superconductors, competition between inter-band and inter-junction Josephson coupling gives rise to frustration and spatial disjunction of superfluid densities among superconducting condensates. Such frustrated coupling manifests as quantum interference of Josephson currents from different tunneling channels and becomes tunable if channel transparency can be varied. To explore these unconventional effects in the prototypical -wave superconductor FeSe, we use atomic-resolution scanned Josephson tunneling microscopy (SJTM) for unprecedented condensate-resolved imaging and junction tuning—capabilities unattainable in macroscopic Josephson devices with fixed characteristics. We quantitatively demonstrate frustrated Josephson tunneling by examining two tunneling inequalities. The relative transparency of two parallel tunneling pathways is found tunable, revealing a tendency towards a 0-π transition with decreasing SJTM junction resistance. Simultaneous visualization of both superconducting condensates reveals anti-correlated superfluid modulations, highlighting the role of inter-band scattering. Our study establishes SJTM as a powerful tool enabling new research frontiers of multi-condensate superconductivity.

Surface Properties of Zirconium diboride (0001) and Homoepitaxial Growth of Zirconium diboride as Determined by Scanning Tunneling Microscopy

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Zirconium diboride (ZrB_2), a group-IV metal-terminated diboride, is an extremely hard material with a high melting point of 3246°C. Thin films of ZrB_2 can be grown conformally via chemical vapor deposition (CVD) using zirconium borohydride, $Zr(BH_4)_4$, as a precursor. Homoepitaxial growth of ZrB_2 was studied using scanning tunnelling microscopy (STM). Exposure of $Zr(BH_4)_4$ to the ZrB_2 (0001) surface at 1400 K led to the formation of ZrB_2 islands. Coarsening of the ZrB_2 islands into layers via Smoluchowski ripening was observed when the islands were left for 60 minutes at 1400 K before imaging at room temperature. In contrast, exposure at 900 K resulted in high-density clusters. Stepwise annealing at 1400 K led to the transformation of these clusters into a continuous thin film via thermal-induced coalescence, with moiré patterns observed as intermediate structures during this coalescence process.

Video-Rate Infrared Camera Based on Solution-Processed Black Phosphorus Films

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Visible-range megapixel cameras are enabled by seamless integration of silicon photodetectors (wavelength <1 μm) and the massively parallel read-out and storage of individual pixel signals by silicon-based complementary metal-oxide-semiconductor (CMOS) integrated circuits. However, alternative materials to silicon are desired for infrared detection beyond $\sim$1 μm; thus, CMOS ROICs must be integrated with a different material with an optical bandgap in mid-infrared. Currently, mid-infrared cameras are fabricated by employing a focal plane array of pixel photodetectors, which are typically made of a III-V or II-VI compound semiconductor, followed by integration with a CMOS ROIC using flip-chip bonding. In this process, an interface material, such as indium, simultaneously provides both electrical and mechanical connections to every pixel detector. However, the intrinsic complexity of this approach imposes significant limitations, ranging from scaling limits to the yield and cost. Nanomaterials with photodetection properties at mid-infrared wavelengths hold promise for high-performance mid-infrared cameras. Solution-processed two-dimensional (2D) materials can be grown, transferred, printed, and patterned directly on CMOS ROICs, eliminating the need for the flip-chip bonding step. In this talk, I will discuss an infrared focal plane array based on the direct transfer of a solution-processed black phosphorus (BP) film onto pre-patterned Si ROIC to achieve photosensitivity extending to mid-infrared wavelengths (>3 μm). Thus, we eliminate the need for flip-chip bonding by developing a method of liquid phase exfoliation that achieves stable dispersions of self-passivated BP flakes. A bottom contact integration of the BP thin film photodetectors with the ROIC chip enables rapid testing of pixel detectors for camera applications. Overall, novel materials processing and transfer allowed the fabrication of FPAs consisting of $>$70,000 functional pixels, where each pixel photodetector exhibits a fast video-rate response time of $<$10 ms and a noise equivalent irradiance below 10^{-4} W/cm^2 at 3.4 μm wavelengths.

Tandem Plasma and Electrochemical Treatment for Near-Complete Defluorination of PFOA

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Per- and polyfluoroalkyl substances (PFAS) are environmentally persistent contaminants that resist conventional water treatment technologies due to the strength of their C-F bonds. Both plasma- and electrochemical-based approaches have shown promise for PFAS degradation, but each has distinct strengths and limitations. In general, degradation by plasmas is much more rapid than electrochemical methods, but is limited by mass transfer effects and less effective with shorter-chain molecules. In this study, we studied the combination of plasma and electrochemical treatment by setting up a tandem configuration. We show that we are able to take advantage of the strengths of both approaches, including the initial degradation of longer chain to shorter chain molecules, followed by more complete degradation of the shorter chain molecules. We initially performed a separate kinetic analysis of a plasma reactor and an electrochemical reactor with perfluorooctanoic acid (PFOA) as a representative PFAS molecule. As expected, plasma achieved more rapid degradation (k_{obs} = 0.06 min^{-1}) than the boron-doped diamond (BDD) electrochemical system (k_{obs} = 0.01 min^{-1}). Both approaches resulted in incomplete defluorination. We then evaluated the tandem plasma-electrochemical system, where a plasma broke down PFOA into shorter chains initially for further degradation by BDD. Transformation kinetics were assessed by liquid chromatography-mass spectrometry (LC-MS) in both synthetic water and real wastewater matrices, and total fluorine balance measurements were used to evaluate the extent of defluorination. The combined system showed more effective treatment performance, particularly in defluorination, reaching $> 90\%$, which was much higher than either the plasma or electrochemical reactors alone. This study demonstrates the synergistic potential of combining plasma and electrochemical strategies for PFAS remediation. Future studies will explore other PFAS beyond PFOA, as well as real mixtures of PFAS containing different chain lengths and functionalities.

Steps Accelerate the Formation of Rhodium Surface Oxide

Maxwell Gillum[1]*, Alexis Gonzalez[1], Elizabeth Serna-Sanchez[1], Allison Kerr[1], Stephanie Danahey[1], Arved Dorst[2], Johannes Diedrich[2], Tim Schäfer[2], Daniel Killelea[1]

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The oxidation of rhodium surfaces has wide-ranging impacts on heterogeneously catalyzed reaction mechanisms. Not only is rhodium itself catalytically active, but it also serves as a robust model system for understanding the oxidation chemistries of platinum-group metals or late transition metals in general. The chemical speciation of oxygen on rhodium surfaces is reasonably well understood and this knowledge can be used to discover how structural changes effect the oxygen speciation. Herein we report our findings for the oxidation of a bifaceted Rh(111)/(322) crystal that shows that when the surface is oxidized the steps hinder the formation of crystalline surface phases at low temperatures and rapid acceleration of surface oxide formation at elevated temperatures. The narrow terraces used provide insight into how highly defective surfaces, like nanoparticles, will behave under strongly oxidizing conditions.

Electric Field-Modulated Atomic Layer Deposition for Modification of Thin Film Properties

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Thermal atomic layer deposition (ALD) has long been used to produce thin, conformal, film growth for microelectronics, photovoltaics, and other industries. Enhanced film properties from thermal processes are required to facilitate continued advancement and downscaling. Electric fields are known to affect gas phase molecules, and adsorption behavior. Common ALD precursors (diethylzinc and water) are modeled using density functional theory to probe the mechanism by which the ALD processes are enhanced. Static electric fields are generated and maintained in situ inside an ALD reactor resulting in modification of film thickness, crystallinity and chemical composition. Thicknesses were determined via spectroscopic ellipsometry, uniformity was investigated by atomic force microscopy, crystallinity by x-ray diffraction, and chemical composition by x-ray photoelectron spectroscopy.

Electrocatalytic-HER Active RuS_2 Thin Films from a New CVD Process

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With the advent of renewable energy and the need for new energy carriers such as hydrogen is pressing. Its production however requires effective catalysts to overcome the high amount of energy currently needed. Ruthenium disulfide, RuS2 has been discussed as promising catalysts in the hydrogen evolution reaction (HER). The commonly accepted descriptor for effective HER is the hydrogen adsorption energy which has been calculated as remarkably low for RuS2 with 0.069 eV. To this day the fabrication of this material has been limited to solution chemical approaches for nanoparticles and sputtering methods for films, and post sulfurization methods of ALD grown films, omitting the advantages chemical vapor deposition (CVD) provides.

A new CVD process using the ruthenium amidinate precursor $Ru(CO)_2(tBuAMD)_2$ and elemental sulfur is presented. The favorable reactivity of the chosen precursor allowed circumventing the use of toxic H_2S often employed in CVD of sulfide films. The resulting polycrystalline thin films were fully characterized by means of XRD, SEM, RBS, NRA, UV/VIS, as well as XPS to reveal promising film properties. The optimal deposition temperature was found to be 600°C on Si(100) substrates enabling homogeneous films with a high degree of crystallinity, and high purity with a near stochiometric Ru to S ratio. To explore the electrocatalytic potential of the herein grown RuS2 films acidic HER experiments were performed. A promising HER activity with a low overpotential of 287 mV for a current of 10 $mAcm^{-2}$ was observed. These proof of principle electrocatalytic studies show that the fabricated RuS_2 thin films are effective HER catalysts and that CVD is a powerful tool which enlarges the accessibility of this pyrite material with a facile process.

Mem-Energy: A Detailed Energy Estimation for Membrane Processes Undergoing Fouling

Nathaniel McNeilly[1,2], Bratin Sengupta[1,3*], Jeff Elam[1*]

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Membrane fouling is a persistent bottleneck in pressure-driven filtration systems, particularly in high-energy applications such as wastewater treatment and oil–water separation. Traditional approaches to evaluate fouling typically rely on pilot-scale testing or complex computational models, which often fail to capture the temporal evolution of flux decline and its direct impact on energy consumption. In this study, we develop a time-resolved, empirical model of membrane fouling using a commercial polyvinylidene fluoride (PVDF) membrane system, with humic acid as a representative foulant. A constant-pressure lab-scale filtration setup was employed to monitor permeate mass over time, revealing a consistent power-law relationship governing flux decay. This relationship enables the formulation of a dynamic transmembrane pressure profile and an associated energy demand model. Leveraging this framework, we conducted a techno-economic analysis comparing unmodified PVDF membranes to metal oxide-coated PVDF membranes engineered via atomic layer deposition (ALD). Over a simulated five-year crude oil–water separation operation, the ALD-modified membranes exhibited significantly reduced energy consumption, highlighting the utility of the model in guiding material selection and process optimization. This work provides a quantitative basis for integrating fouling dynamics into membrane performance evaluations and supports energy-efficient design of next-generation filtration systems.

Probing the Growth Mechanisms of ALD on Chemically "Inert" Polymers

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Atomic layer deposition (ALD) is a self-limiting, conformal thin-film growth technique widely employed in semiconductor manufacturing, and increasingly in applications such as catalysis, energy storage, water purification, and membrane technologies. In many of these emerging areas, device flexibility and compatibility with polymeric substrates are critical. While polymers offer unique advantages, including surface and subsurface deposition capabilities, many commonly used polymers—such as Polyvinylidene Fluoride (PVDF), Polytetrafluoroethylene (PTFE), and Polypropylene (PP)—have been considered chemically "inert," limiting their exploration. Prior studies have attributed ALD growth on these substrates to diffusion and physical entrapment of precursors rather than true chemical interactions. Here, we report notable evidence of chemical bonding between ALD precursors and these "inert" polymers, despite the apparent absence of reactive surface functionalities. In situ and ex situ characterizations reveal precursor-polymer bond formation, indicating that ALD may enable chemical modification of such polymers. These findings challenge the conventional understanding of ALD on "inert" substrates and open new avenues for enhancing polymer functionality in applications such as hydrophilic membrane coatings and polymer-based energy devices.

Contributed Posters

Structural Study of Rhodium Based Metal Surfaces

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Heterogeneously catalyzed oxidation reactions, such as the catalytic process of converting CO to CO_2, are extensively utilized for the production of modern commodities. However, there is little information known about the atomic level details of these catalytic processes. In order to further our understanding of the process at an atomic level, the investigation herein will focus on characterizing structures of oxygen on Rh model catalysts. Scanning tunneling microscopy (STM) images illustrate how the behavior of oxygen is affected by features such as surface defects and step width. Alongside the STM, other techniques such as temperature programmed desorption (TPD), and low energy electron diffraction (LEED) are used to identify the various species of oxygen and the structures they form on the surface.

Observation of Persistent Zero Modes and Superconducting Vortex Doublets in UTe_2

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Superconducting vortices can reveal electron pairing details and nucleate topologically protected states. Yet, vortices of bulk spin-triplet superconductors have never been visualized at the atomic scale. Recently, UTe_2 has emerged as a prime spin-triplet superconductor, but its superconducting order parameter is elusive, and whether time-reversal symmetry (TRS) is broken remains unsettled. Here, we visualize vortices on the (011) surface of ultra-clean UTe_2 single crystals (T_c=2.1 K) using scanning tunneling microscopy (STM). We introduce $\frac{d^2I}{dV^2}$ imaging as an effective technique for vortex visualization in superconductors with substantial residual zero-energy density of states (DOS), as in UTe_2. Anisotropic single-flux-quantum vortices, with coherence lengths of $\sim$12 nm (4 nm) parallel (perpendicular) to the a-axis, form a triangular vortex lattice (VL) under a small out-of-plane magnetic field. The invariance of vortex structures and VL under changes of field polarity and cooling history strongly supports time-reversal invariant superconductivity under zero field. At vortex cores (VCs), non-split, spectrally sharp zero-bias conductance peaks (ZBPs) persist up 8T that are consistent with symmetry-protected Majorana zero modes (MZMs) in a topological vortex line. Close examination of vortex structures reveals a mirror-asymmetric doublet—one with ZBPs and another with an enhanced superconducting gap, possibly originating from a field-induced multi-component order parameter.

Tip-enhanced Raman Spectroscopy in Probing Metal Surface Reactivity Towards Charged Species and Organic Ligands

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Understanding the reactivity of metal surfaces at the molecular level is pivotal for advancing catalysis, electrochemistry, surface functionalization, and nanomaterials science. In this work, Tip-Enhanced Raman Spectroscopy (TERS) has been employed to investigate the local chemical environment and surface interactions of charged species and organic ligands on reactive metal substrates with sub-nanometer-scale spatial resolution. TERS uniquely enables vibrational fingerprinting under ambient and operando conditions, providing both chemical specificity and topographic context. By combining the chemical sensitivity of vibrational spectroscopy with the spatial precision of scanning probe techniques, UHV-TERS enables direct observation of adsorption geometries, ligand-surface bonding motifs, and charge transfer dynamics with nanometer-scale resolution. Our measurements reveal distinct interaction pathways and surface selectivity based on ligand structure and charge state, with implications for stability, electronic coupling, and reactivity. In particular, we highlight how local electronic environments influence the anchoring and deformation of N-heterocyclic carbene (NHC) and porphyrin ligands, and how the adsorption of $[\mathrm{Ru(bpy)_3}]^{2+}$ is modulated by its charge distribution and surface potential on noble and transition metal surfaces. By correlating Raman spectral features with scanning probe microscopy data, we reveal distinct site-specific reactivity patterns that govern surface chemistry at the molecular scale.

Methanol dehydrogenation on Pt / Cu (111) single atom alloy surface

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Pt/Cu(111) single atom alloy s (SAAs) have been reported to catalyze the non-oxidative dehydrogenation of alcohols, selectively forming the corresponding aldehydes and hydrogen. They do so by facilitating O-H bond cleavage to form an alkoxy intermediate and C-H bond cleavage of the alkoxy to form the aldehyde. In this study, methanol dry dehydrogenation reactions on Pt/Cu(111) SAA surfaces were investigated using reflection absorption infrared spectroscopy (RAIRS) and temperature programmed desorption (TPD) to determine reaction intermediates and pathways. Although no formaldehyde desorption was observed from Cu (111), 0.02 ML of formaldehyde desorbs from a Pt/Cu (111) surface at 375 K. A RAIRS peak at 1005 cm^{-1} on the SAA surface, observed at 250 K, was assigned to the C–O stretching mode of methoxy, compared to the corresponding methoxy C–O stretching peak (1005 cm^{-1}) on an oxygen-pre-adsorbed Cu (111) surface. The methoxy yield (0.001 ML), estimated from the CO stretching peak area on the SAA surface, was lower than the number of Pt single atoms (0.04 ML), contrary to the expectation that a single Pt site could form multiple methoxy molecules via spillover onto Cu sites. To assess the effect of background CO, the formaldehyde yield was compared to an SAA surface where Pt sites were blocked by CO dosed at 250 K. The formaldehyde yield decreased by approximately 50%, confirming that background CO suppresses the reaction yield on the Pt/Cu (111) SAA surface. These findings provide insights into the mechanistic role of Pt sites in methanol dehydrogenation and the impact of surface species on catalytic efficiency.

The Role of Multiparticle Interactions in Diffusivity and Site-Specificity of Binding on Moiré Patterned Graphene

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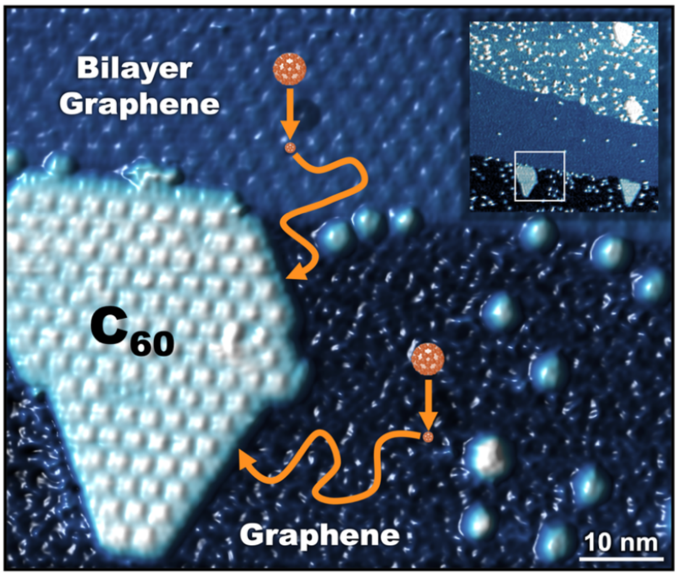
The moiré pattern of epitaxial graphene on Ru(0001) presents a palette of binding sites for atomic and molecular species. STM topography reveals the site-specific binding and diffusivity of atomic oxygen across the moiré. Side-by-side comparison of monolayer and bilayer graphene on Ru(0001) illustrates the importance of spin-forbidden dynamics of O(3P) scattering onto graphitic surfaces. Meanwhile, multiparticle interactions lead to correlated motion and higher diffusion rates of oxygen atoms on the surface. Similarly, physical vapor deposition of buckminsterfullerene (C60) on Graphene/Ru(0001) results in a time evolving interface where individual C60 molecules coalesce into larger islands.O(3P) adsorption before dosing C60 disrupts ordered film formation and leads to less mobile C60 molecules on the surface at room temperature. The effects of supersonic O(3P) on C60/graphene/Ru(0001) are additionally visualized via STM. Overall, results lend insight to the synthesis and stability of moiré templated two-dimensional materials which show promise as next-generation platforms for quantum materials and catalysts.



Reactions of Atomic Hydrogen with Surface-Oriented Even and Odd Chain Length Brominated Self-Assembled Monolayers

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We have conducted a spatially and angle-resolved investigation of the on-surface products of reactive scattering from a directed H atom beam. Self-Assembled Monolayers (SAMs) of 11-bromoundecanethiol (11-Br), 12-bromododecanethiol (12-Br), decanethiol (10C), and mixtures thereof were prepared on Au(111) and reacted at room temperature with H atoms from an effusive atomic beam at 2000 K. The role of collisional orientation between the primary bromine and hydrogen atom was examined in the context of the debromination rate. Due to the odd-even effect, collisions of H atoms with the terminal bond of 11-Br occur at an average of 130° while collisions with 12-Br occur at an average of 105°. Debromination reaction rates were monitored with STM and XPS. STM analysis used SAMs composed of 95%/5% 10C/11- or 12-Br, as well as films composed purely of 11- or 12-Br, while XPS used only pure films of 11-Br, 12-Br, or 10C. 11-Br was found to be 13% more reactive than 12-Br with reaction probabilities of $P11 = (1.03 \pm 0.02)\%$ and $P12 = (0.91 \pm 0.04)\%$ with respect to the average number of H collisions determined from the STM data of dilute brominated alkane films in 10C. It was observed in the STM data for pure films of brominated alkanes that debromination occurs primarily from the interior of SAM domains as well as from the domain grain boundary. The XPS data of pure 11-Br, 12-Br, and 10C films indicated that direct debromination of the terminal carbon is the primary pathway for bromine to leave the surface. It was concluded that the debromination pathway is favored by direct collisions between the H and Br atoms. The use of brominated alkanes presents itself as an effective method to passivate gold against H atoms in comparison to a fully hydrogenated SAM of equivalent length. These studies with surface-oriented molecules present a complementary route for examining geometry-constrained molecular reactivity, joining more traditional gas phase studies that have used either orienting fields or optical alignment to address similar questions.

CO and CO_2 on Rh(111) Surface

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The adsorption of CO and CO_2 on transition metals has been widely studied due to their importance as benchmark molecules in surface science, where they are used to probe metallic surfaces through the electronic structure and surface reactivity changes they introduce. Using Density Functional Theory calculations within the Vienna Ab Initio Simulation package (VASP), we calculated the binding energies of CO and CO_2 at different sites on the Rh(111) surface. Three different exchange-correlation functionals were employed to treat electron-electron interactions: Perdew-Burke-Ernzerhof (PBE), vdW-DF2, and optB86b-vdW functionals. The latter two include non-local correlation effects to capture dispersion interactions. In addition, we explored CO_2 decomposition into CO and O using these functionals. Finally, vibrational frequency calculations were performed for CO adsorbed on both the clean Rh(111) surface and the surface with subsurface oxygen to validate the structural stability of the optimized configurations. The calculated frequencies are compared to experimental observations and previous computational results to establish the accuracy and reliability of our theoretical approach.

XPS Study of Initial Oxygen Adsorption on ZrB_2 (0001) at Room Temperature

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Zirconium diboride (ZrB_2) is an ultra-hard material with a melting point of 3246°C, making it suitable for extreme environment applications such as hypersonic vehicles and cutting tools. Understanding its interactions with molecular oxygen (O_2) is crucial for predicting its performance. This study investigates the nascent stages of oxygen uptake on the ZrB_2(0001) surface at room temperature. A clean, well-ordered ZrB_2(0001) surface, confirmed by a characteristic (1x1) low energy electron diffraction (LEED) pattern, was exposed to O_2 dosages ranging from 0.01 to 1.0 L. X-ray photoelectron spectroscopy (XPS) was employed to track the evolution of surface composition. Analysis of the O 1s spectra following even minimal exposures reveals multiple distinct oxygen species. Two primary components were identified: one at a binding energy of 533.8 eV corresponding to oxygen adsorbed on the surface, and another at 531.4 eV attributed to oxygen incorporated into the subsurface region. These findings indicate that even at very low O_2 exposures at room temperature, oxygen not only dissociatively adsorbed onto the ZrB_2(0001) surface but also begins to penetrate the subsurface layers. This work demonstrates the capability of XPS to distinguish initial surface and subsurface oxygen species on ZrB_2(0001). The observation of subsurface oxygen at room-temperature exposures provides critical experimental data for understanding the onset of its oxidation pathway.

Selective Hydrogenation of Styrene to Ethylbenzene Over a Pd/Cu(111) Single-Atom-Alloy Surface

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The selective hydrogenation of styrene to ethylbenzene is of industrial significance due to its role in purifying xylene-rich streams used for para-xylene production, a key precursor to polyester fibers and PET plastics. Trace styrene can disrupt downstream separation and catalytic processes, especially in adsorptive purification systems. However, achieving high selectivity is challenging, as conventional catalysts often induce aromatic ring hydrogenation or xylene isomerization. Catalysts that can selectively hydrogenate the vinyl group while preserving the aromatic core are therefore essential. Single-atom alloy (SAA) catalysts have emerged as promising candidates for such transformations. In these systems, small amounts of an active metal are atomically dispersed in a less reactive host. The isolated active atoms serve as active hydrogen dissociation sites, while the surrounding relatively inert atoms suppress undesired over-hydrogenation. This ensemble effect enhances chemo-selectivity and reduces precious metal usage, making SAAs attractive platforms for probing structure–reactivity relationships in hydrogenation catalysis. In this study, we investigated the hydrogenation of styrene to ethylbenzene over a Pd/Cu(111) SAA under ambient pressure using reflection absorption infrared spectroscopy (RAIRS). The appearance of gas-phase ethylbenzene peaks below 3000^{-1} (due to sp^3 C–H stretches) and the loss of the styrene vinyl bending mode at 909 cm^{-1} confirm successful hydrogenation. Auger electron spectroscopy (AES) of the post-reaction surface revealed carbon deposition, suggesting some dissociation. No spectral features associated with cyclohexyl ethylbenzene were detected, indicating high selectivity. The reaction showed 100% conversion with excellent selectivity toward ethylbenzene. A turnover frequency (TOF) of 46 s^{-1} at 380 K was observed, significantly higher than that for pure Cu, confirming the role of Pd sites. The activation energy was determined to be 32 ± 4 kJ/mol. Further kinetic investigations and in-situ identification of surface-bound intermediates via RAIRS are currently in progress.

Energy-dependent Sticking Probabilities of Carbon Dioxide Isotopologues Under Non-Equilibrium Gas-Surface Collision Conditions

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The process of non-equilibrium gas-phase condensation remains poorly understood, particularly in regard to the fundamental mechanisms that govern energy exchange at surfaces. This dynamic phenomenon involves gas molecules colliding with an interface and losing energy through adiabatic or non-adiabatic interactions, which in turn influence condensation behavior. The rate and efficiency of condensation are determined by a range of factors, including the kinematics of incident particles, interfacial phonon density of states, and the characteristics of nucleation sites. Despite longstanding interest in non-equilibrium condensation, critical gaps persist, especially concerning how energy dissipation affects energy accommodation at the surface. These processes are especially relevant in astrochemical environments such as the interstellar medium (ISM), where gas-surface interactions on dust grains play a key role in molecular formation. Isotopic mass differences can lead to varying condensation rates, producing distinctive isotopic signatures that offer insights into the ISM's chemical evolution. Understanding energy transfer in isotopically selected systems also informs practical phenomena like aircraft icing in cold atmospheres. In this study, we present a combined molecular beam and Molecular Dynamics investigation of the sticking behavior of two CO_2 isotopologues, $^{12}CO_2$ and $^{13}CO_2$, across a range of incident energies. Experimental results, obtained using King and Wells mass spectrometry alongside in situ reflection absorption infrared spectroscopy (RAIRS), reveal isotopologue-dependent sticking probabilities on pre-condensed CO_2 films.

Engineering Ion Transport in Nanochannels for Energy-efficient Neuromorphic Computation

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The advent of AI and machine learning offers unprecedented potential to address global challenges, but it comes with an escalating demand for computing power and energy consumption. The need for energy-efficient computing mechanisms is more pressing than ever, and we can look to the brain for inspiration on co-localized computation and memory for highly efficient information processing. Emulating the brain in synthetic systems requires a deeper understanding of the ion transport mechanisms and device characteristics required to achieve this goal. Promising devices include memristors that integrate their history of applied currents and voltages to affect their future conductance in a process that mimics the propagation of signals across neurons via changes in synaptic strength. This research explores how asymmetrically charged nanochannels can be tuned to exhibit memristive neuromorphic plasticity. To achieve this, we will fabricate a device with charge-Janus properties through advanced lithography techniques and functional coatings. These charge asymmetries will be characterized and confirmed through x-ray photoelectron spectroscopy and zeta potential measurements, while current-voltage sweeps across varying electrolyte compositions and concentrations will probe the system's memristive hysteresis. Voltage pulse sequences can be applied to evoke neuromorphic Hebbian learning which could be integrated with a single-layer neural network to perform logic. Through this work, we will be able to uncover mechanisms of asymmetric ion transport in nanochannels to aid the development of energy-efficient, brain-inspired computing architectures, and it will also support advancements in chemical separation and sensing applications.

Metal-Insulator Transition in $CaVO_3$ thin films

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Thin films of $CaVO_3$ are observed to undergo an MIT as a function of film thickness. Thin films of $CaVO_3$ with thicknesses of 90 u.c., 45 u.c., 30 u.c., 20 u.c., and 15 u.c. on an $SrTiO_3$ substrate were measured by ARPES, and changes in the electronic structure were tracked. The observed changes in the Fermi surface point towards increased tensile strain on the film as the thickness is decreased. A decrease in conduction band bandwidth and an increase in V3+ states in thinner films were observed, indicating the localization of electrons near the Fermi level. An MIT was observed when transitioning from a metallic 20 u.c. film to an insulating 15 u.c. film, with the disappearance of the conduction band and the appearance of an insulating flat band at $\sim$ -0.9 eV. We conclude that the increased epitaxial strain, rather than dimensionality, is the driver of the MIT, in agreement with previous studies.

Oxidation Studies of Au Capped Nb Surfaces

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Nb is the highest temperature elemental superconductor; however, its application in particle accelerators and quantum computers is limited by growth of lossy insulting oxide layers. Au capping layers have been shown to improve accelerating performance but Au morphology, kinetics, and degree of passivation at various coverages on Nb have not been fully investigated. This work characterizes the physical deposition and oxygen contamination of sub-ML to 10 ML Au coverages on different Nb surfaces. We analyze the physical features and chemical states of the surface using Scanning Tunneling Microscopy, X-ray and UV Photoelectron Spectroscopy, and Auger Electron Spectroscopy. Results show that annealing treatments as low as 350° C causes Au de-wetting and island formation at Sub-ML to 10 ML coverages, substantially exposing Nb to oxidation. Further investigation is needed to reveal the optimal method to passivate Nb.

Modeling and Characterization of Microwave-powered, Atmospheric-pressure Plasma Reduction of Iron Oxide

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Plasma-based approaches to iron oxide reduction have attracted attention to expand the possible raw ores and gaseous feedstocks that can be reacted. While reduction has been demonstrated, the fundamental mechanisms are complicated by the interplay of reactions and diffusion. Compared to a thermal process, a mixture of species are generated in a plasma, including radical intermediates such as atomic hydrogen. In this study, we set up a simplified experiment to study plasma reduction of iron oxide. Sintered disks were fabricated from powders of hematite with controlled porosity. The disks were then treated with a plasma formed as a jet impinging at the surface. The plasma was characterized by optical emission spectroscopy to determine densities of radicals such as atomic hydrogen. Following reduction, the disk was characterized by various techniques to determine the extent of reduction, including as a function of distance from the surface into the bulk. Experiments were supported by a reaction-diffusion model.

Understanding Interfacial Structure to Enhance Electrochemical Capacitance in Ionic Liquid Electrolytes

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Growing use of intermittent wind and solar energy necessitates research into new materials and devices that can compensate grid-scale power fluctuations. This creates a new role for high power density supercapacitors that quickly charge and discharge excess electrochemical energy. An ideal supercapacitor electrolyte has a wide electrochemical stability window and high capacitance to maximize energy density. Ionic liquids (ILs) show potential as supercapacitor electrolytes with their wide electrochemical stability windows, nonflammability, and nonvolatility. Yet, pronounced ion-ion correlations present in ILs often result in low capacitances, particularly at large voltages. I will discuss our work aimed at tuning ionic correlations in IL blends to provide pathways towards higher energy density capacitive interfaces. We find that mixing surface-active amphiphilic anions into ILs doubles the capacitance at negative surfaces. Therefore, we hypothesize that anion-anion van der Waals interactions weaken IL cation-anion interactions and drive molecular assembly at negative surfaces, increasing capacitance. We also observe that co-ions, or ions of same charge to the surface, play an equivalent role to counterions, ions of opposing charge to the surface, at dictating interfacial capacitance in IL mixtures. We then investigate the interfacial structure of ionic liquid mixtures using surface forces measurements to understand the mechanism behind increased capacitances. Ultimately, these investigations inform the role of co-ions and mixture entropy at promoting self-assembly to design higher energy density ionic liquid electrolytes for supercapacitors.

Surface Sterilization versus Disinfection Using LED Ultra-Violet C irradiation – A Study of Reproducibility & Accuracy

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Anti-Microbial Resistance kills 50,000 patients/year in the US, 1.3 Mil /year globally, and is projected to surpass cancer as leading cause of death by 2050. Since 2010, viral outbreaks have occurred ∼2 years, twice the historical rate: H1N1 (2009), MERS (2012), Ebola (2014), Zika (2015), and Covid-19 (2019). Sterilization, per FDA, means reducing the probability for a single viable microorganism to less than 10^{-6}, defined as Sterility Assurance Level (SAL) of 6. Standard sterilization methods aren't usable in public and hospital spaces. UVC irradiation eradicates pathogens by breaking bonds in nucleic acid pairs in DNA/RNA and is used in disinfection (SAL = 3). The present study investigates $260-280$ nm LEDs to sterilize surfaces beyond disinfection using Lactobacillus Acidophilus (Lacto. A). The LEDs deliver a power density of 0.8 ± 0.04 mW/cm^2 at a distance of 1 cm. For reproducibility and accuracy, two studies A and B used three identical sets of 10 cultures, including a control. Seeding with calibrated Lacto. A. produced CFU counts within one order of magnitude: $50\pm(25\times10^6)$ for A and 500×10^6 CFU/mL for B, typical for microbial cultures reproducibility. After serial dilution, A and B are inoculated. The control, 'No UVC' is compared to the 2 sets irradiated for 180 s; the other half is left unirradiated to account for variations in culture growth. Irradiation for 180 s yields an energy density 144 ± 7 mJ/cm^2 on a 4 cm^2 square area yields an average kill rate of 99.9993% on surfaces per repeated CFU counting, with reproducibility with half an order of magnitude. In conclusion, UVC LEDs can consistently reach SALs above 3, achieving SALs of 5. Energy density at 1 cm must be increased by a factor of 5 to achieve sterilization with a SAL of 6.

Toward Selective Metal Deposition on Dielectrics: Exploring Inhibitor Choices and a New Strategy

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Metal-on-dielectric (MoD) structures are critical in advanced microelectronics, where precise metal patterning on dielectric layers is essential. However, achieving selective metal growth on dielectric surfaces within a single process remains a significant challenge. We propose a novel strategy to control the selective growth of metal thin films on dielectric surfaces. This approach is based on atomic layer deposition (ALD), a promising technique for MoD coatings due to its self-limiting surface reactions, excellent conformality, and precise thickness control. We introduce an inhibitor pulse prior to the metal ALD process to prevent metal precursor adsorption, thereby enabling selective metal film growth on targeted dielectric surfaces. In this work, we investigate and compare the performance and trade-offs of two inhibitors: butyraldehyde (BTA) and bis(N,N-dimethylamino)dimethylsilane (DMADMS), for controlling the selective growth of ruthenium (Ru) metal thin film on an Al_2O_3 – SiO_2 dielectric system. The Ru ALD process utilizes a novel precursor, $(C_4H_6)Ru(CO)_3$, with O_2 as the reactant. The adsorption behavior of BTA and DMADMS, along with the selectivity of Ru film growth, is characterized using water contact angle (WCA) measurements, ellipsometry, and X-ray photoelectron spectroscopy (XPS). Our findings offer an innovative and effective strategy for bottom-up 3D patterning in MoD applications and advanced semiconductor manufacturing.

Strain-engineered Spin-exciton Coupling in Two-dimensional Magnetic Semiconductor

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Two-dimensional (2D) materials allow the exploration of previously inaccessible basic physics phenomena in low dimensions. In particular, 2D magnetism has emerged as a promising platform for developing novel magneto-optical, magnetoelectric, and spintronic devices. Among 2D magnetic materials, CrSBr—an anisotropic, air-stable, magnetic semiconductor [1]— has garnered significant attention for its stable exciton, magnetic order bound to its lattices. These intertwined degrees of freedom give rise to rich light-matter interactions including exciton-magnon coupling [2], exciton-lattice interaction [3] and cavity-enhanced polariton [4]. Importantly, such quantum phenomena can be tuned through external control of magnetic order and lattice strain, offering both fundamental insights and practical utility for device applications [5]. However, its excitonic responses—especially those governed by local strain and spin order—remain largely unexplored.

In this work, we investigate excitonic behavior induced by localized strain in CrSBr. Few-layered CrSBr flakes were transferred onto pre-patterned SiO_2/Si substrates containing cylindrical and rectangular trench structures, inducing spatially varying uniaxial or biaxial strain in the range of 0.1–1%. Using optical spectroscopy and scanning probe techniques, we correlate the polarization dependent excitonic responses to both local strain and spin order. Our results reveal that the spin configuration is influenced by strain, which, in turn, affect the excitonic photoluminescence. These findings highlight the potential of strain engineering in controlling spin-exciton interactions in 2D magnetic semiconductors and open new opportunities for quantum transduction at the atomically thin magneto-optoelectronic devices.

Acknowledge statement

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Anisotropic Defect Hopping in FeSe

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Electronic nematicity is most frequently considered in its impacts on electron-scale properties (e.g. anisotropic resistivity) but it remains an open question as to the energy scale electronic nematicity impacts. Scanning tunneling microscopes (STM) have been used to induce atomic defect movement in a variety of systems. Here we demonstrate anisotropic STM induced atomic-defect hopping in FeSe, a system with anisotropy arising from its electronic nematicity. This anisotropy is an atom-scale property exhibited at energies of hundreds of meV, an energy higher than other reported nematicity signatures.

Towards Long-term Operation and Scale Up of Plasma-liquid Reactors for Nitrogen Fixation

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Plasma-based chemical approaches to nitrogen fixation have received a resurgence of interest because of the ability to react molecular nitrogen at atmospheric pressure using electricity and without any external heating. One example of a reactor is a plasma formed in contact with liquid water in which products are synthesized as dissolved ions such as nitrate, nitrite, and ammonium. Such an approach has potential to provide fixed nitrogen in an easily transportable and deliverable form for plants or microorganisms.

In this project, we are interested in long-term operation and scalability of a plasma-liquid process for fixing nitrogen. Studies were carried out on two reactors. First, we performed parametric studies on a single plasma in contact with liquid water and monitored fixed nitrogen production over time. In general, the production rate was found to rapidly decrease in the first hour. Efforts to understand and keep the rate high will be presented. Second, we designed and tested a large-scale reactor made up of multiple plasmas and overall increased power and volume. Scaling of production rates with these factors was assessed and will be discussed. Overall, this work provides a path to implementing plasma technology in future agricultural and biotechnology applications.

4D Spatial Biology of Viral Infection: New Methods for Therapeutic Target Identification

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While the Covid19 pandemic was a tragedy on a massive scale, and a vaccine was developed in a record time frame, our society suffered massive losses. In addition to the huge losses of life, Infrastructure suffered from differing patterns, the wounded economy is still recovering, and we are still learning about the consequences of the isolation of lock-down. One point has been made abundantly clear during these events; we are not ready for the emerging threats of worldwide pandemics. We need better tools to combat pathogens and develop responsive therapeutics to future health emergencies. Our lab is a part of a much larger group designing and collaborating on a project coined “4D spatial biology”, which will be an integrated workflow of cutting-edge molecular biology and imaging techniques with the intent of accelerating the identification of pathogenic countermeasures. This project will combine Lattice Light Sheet Microscopy (LLSM) to capture the sequence of infection events with subsequent molecular analysis using cryo-electron tomography (cryoET), cryo-NanoSIMS, and Spatial Transcriptomics. To promote this effort, we are developing the workflow for cryo-NanoSIMS, and partially for the LLSM. We are employing flu virus strains with different morphologies that are thought to influence their infectivity as a test case for the 4D spatial biology workflow. I am developing fluorescent and isotopically labeled virus particles and to incorporate distinct stable isotopes into specific membrane components in the host cells to allow tracking the roles of these components with NanoSIMS. The fluorescent and isotopically labeled virus will allow tracking virus infection with LLSM and cryo-NanoSIMS, whereas the host cells that contain rare isotope-labeled membrane components will allow visualizing key metabolites during events of interest using cryo-NanoSIMS for the first time. Progress towards these goals will be presented.

Visualizing Membrane Protein Dynamics in Phaeodactylum tricornutum–Bacteria Co-cultures

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Bacterial attachment influences the viability of algal cells and their ability to convert solar energy and CO_2 into valuable products. We hypothesize that the lipid and protein distributions in the algal cell membrane is a readout for the nature of bacterial interactions, distinguishing between beneficial, commensal, and parasitic bacteria. To test this hypothesis, we are developing the ability to image specific membrane proteins and lipids in the membranes of the marine algae, Phaeodactylum tricornutum (Pt), with $\sim$10 nm lateral resolution using a Cameca NanoSIMS. Because each component of interest must contain a rare isotope or nonnative element to permit its detection with a NanoSIMS, we sought to fuse a protein in the Pt membrane to a self-labeling enzyme, SNAP-tag or HaloTag. These tags selectively react with small substrates that may be functionalized with a reporter. They are routinely fused to proteins of interest in mammalian cells, allowing selective labeling of the protein of interest. We demonstrate for the first time that SNAP-tag and HaloTag enable the selective labeling of target proteins in algae. Episomal plasmids for expression of SNAP-tag or HaloTag fused to a Pt membrane protein, the bicarbonate transporter protein SLC4-2, were constructed and introduced into Pt via trans-kingdom conjugation. Functional SNAP-tag and HaloTag expression in Pt was confirmed by labeling with fluorescent substrates and fluorescence microscopy imaging. This system was used to investigate whether bacterial attachment to Pt alters SLC4-2-SNAP-tag protein distribution in the Pt membrane. Ongoing work involves developing a SNAP-substrate that may be detected with NanoSIMS, and combining it with NanoSIMS imaging to probe whether the attachment of beneficial, commensal, or parasitic bacteria induces changes in protein distribution in the Pt membrane. This would be a direct test of the hypothesis that membrane protein distribution is a readout for the nature of the bacteria-algae interaction.

Monitoring of Ice Premelting at the Buried Ice-Polymer Interface with the Quartz Crystal Microbalance

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Premelting of ice, the formation of a quasi-liquid water layer at the surface of ice below the bulk melting point, is poorly understood but instrumental in understanding interactions at the ice surface. We present a study of premelting using a quartz crystal microbalance (QCM) to acoustically probe the quasi-liquid layer (QLL) at the buried ice-substrate interface. We demonstrate the ability of the QCM to measure water premelting at a range of temperatures for ice-surface interfaces with both the bare gold electrode of the QCM and polymer thin films.

Synthesis and Postprocessing of Atomic Layer Deposition (ALD) Grown MoS_2 Thin Films

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Atomic-layer-deposited (ALD) MoS_2 provides wafer-scale, angstrom-level thickness and composition control for ultra-low-power electronic applications. However, as-deposited ALD MoS_2 is amorphous, defect-rich, and rapidly accumulates ambient contaminants that degrade electrical performance. We investigates sub-2 nm ALD MoS_2 films on Si/SiO_2 alongside co-deposited sulfurized Mo metal films. In-situ spectroscopic ellipsometry monitored surface uptake during controlled ambient exposure immediately after deposition. A two-step post-processing sequence was evaluated: a forming-gas anneal (FGA, 250-300°C for 30-45 min) to desorb adventitious species, reduce near-surface oxides, and replenish sulfur at defects; followed by a high-temperature H_2S anneal (800-900°C for 30-75 min) to drive sulfurization and crystallization. Variants FGA+H_2S, H_2S-only, and Mo metal sulfurization isolated the roles of cleaning, sulfur replenishment, and crystallinity on electrical transport.

Ellipsometry kinetics reveal gradual, continued thickness growth ($\sim$ 0.4 nm) on amorphous MoS_2 due to defect-mediated oxygen passivation and adsorbate uptake, whereas Mo metal forms a rapid, self-limiting MoO_x layer ($\sim$ 0.25 nm). Raman spectroscopy confirms the transition from broad, defect-rich bands to sharp $MoSi_2$ vibrational modes after optimized annealing. Four-point-probe measurements demonstrate strong resistivity, further driving the need for more optimized post-processing. These results define process windows for integrating ultrathin, electrically functional $MoSi_2$ into memristor and FET architectures, advancing scalable, energy-efficient microelectronics.

Atomic Layer Deposition of p-type Molybdenum Disulfide ($MoSi_2$) for Microelectronics

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Molybdenum disulfide (MoS_2), a two-dimensional semiconductor, is a promising next-generation alternative to silicon in microelectronics due to its direct band-gap at monolayer thicknesses and inherent scalability. A significant challenge hindering its application is the reliable p-type doping required for fabricating complementary logic devices. While this has been demonstrated using Plasma-Enhanced ALD (PEALD), a robust and scalable thermal ALD process for p-type MoS_2 remains a key, unaddressed challenge.

In this study, MoS_2 thin films were grown and doped in-situ with aluminum via thermal ALD. The resulting films were characterized by in-situ ellipsometry to monitor growth, while X-ray Photoelectron Spectroscopy (XPS) depth profiling and Hall measurements were used to determine chemical composition and electrical properties, respectively.

We successfully demonstrate the conversion of intrinsically n-type MoS_2 to p-type. XPS analysis confirmed that the aluminum dopant was distributed throughout the entire film thickness. A clear trend was observed where increasing aluminum doping leads to an increased p-type bulk carrier concentration and a corresponding decrease in mobility, demonstrating fine control over the film's carrier concentration and mobility. However, a 1:16 ratio was insufficient to overcome the material's intrinsic n-type behavior. This controlled doping is a critical step towards the realization of MoS_2-based p-n junctions and other functional 2D electronic devices.

Electrochemical Oxidation of PFAS using Bi_2O_3-SnO_2 deposited Reactive Electrochemical Membranes and Development of PFAS Oxidation Selective Anodes

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Foam fractionation or the use of ion exchange resins (IXR) are effective methods to treat per- and polyfluoroalkyl substances (PFAS)-contaminated groundwater, but these methods produce concentrated PFAS waste. Electrochemical oxidation of PFAS using Ti_4O_7 reactive electrochemical membranes (REMs) has been demonstrated to effectively oxidize PFAS in some matrices and is a potential method for mineralizing concentrated PFAS waste. In this work, we focused on the synthesis of Bi_2O_3-SnO_2 electrocatalyst using electrodeposition on REMs to further enhance the reaction rates of PFOA oxidation. The synthesized electrocatalytic REMs were characterized using X-ray photoelectron spectroscopy (XPS) to evaluate the composition and oxidation states of the electrocatalyst. Moreover, top surface and cross-sections of the REMs were mapped using scanning electron microscopy energy dispersive X-ray spectroscopy (SEM-EDS). The synthesized REMs were then tested for electrochemical oxidation of $\sim$41 mg L^{-1} perfluorooctanoic acid (PFOA) in a flow-through reactor at a constant potential and flux in $NaClO_4$, Na_2SO_4, NaCl, and $(NH_4)_2SO_4$ electrolytes. Also, electrochemical oxidation of PFAS was tested in the groundwater matrix and IXR still bottoms solution. The permeate collected from oxidation experiments was analyzed for long- and short-chain PFAS using liquid chromatography tandem mass spectroscopy and fluoride production using ion chromatography. Short-chain PFAS (C2, C3, C4, C5, C6, C7) were detected with 10-25% yield, along with the formation of fluoride with 60-80% yield. Moreover, the samples were analyzed using inductively coupled plasma mass spectroscopy to assess the leached electrocatalyst under anodic conditions. The work also focused on the use of atomic layer deposition (ALD) for synthesizing PFAS-selective anodes. For the development, the use of silanes along with an insulating layer (Al_2O_3, TiO_2, AlF_3, and SiO_2) was proposed for vapor phase grafting on the anodes to suppress the oxygen evolution reaction (OER), which is a side reaction under anodic conditions.

Vacuum Characterization Techniques to Elucidate Water Electrolyzer Degradation Mechanisms

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A major barrier currently preventing more economical anion exchange membrane water electrolyzers (AEMWE) from being used in industry for green hydrogen production is low durability. To improve membrane durability, the chemical and physical processes leading to the rapid degradation of the membranes must be uncovered. For this reason, we are characterizing the chemistries and morphologies of anion exchange membranes (AEM) before and after failure to identify the changes in the material that lead to a drop in performance. The main areas of examination are hydroxide ion conductivity and membrane durability. We are using scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDS), X-ray photoelectron spectroscopy (XPS), and secondary ion mass spectroscopy (SIMS) to examine the morphological and chemical composition changes of the material. Specifically, SEM-EDS images of surface morphology and composition show qualitative changes after operation. Software can help give a quantitative analysis for further comparison of surface changes. Information on chemical bonds within the material at the surface or in a depth profile has been acquired with XPS, and the data provides insight into the chemical reactions that may have taken place. SIMS has been employed to investigate surface composition and used to acquire depth profiles of the material. A computational depth correction approach has been applied to the SIMS depth profiling data to create more accurate three-dimensional images of the material's composition. These efforts are expected to shed light on the degradation mechanisms in anion exchange membranes. Elucidation of these degradation mechanisms may lead to the synthesis of more stable membranes, providing the economic viability needed to make AEMWEs an industrial technology for green hydrogen generation.

New Polar Quantum Materials - Controlling Ferroelectricity and its Interaction with the Environment

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Twisting transition metal dichalcogenide (TMD) layers in the limit of very small angles, relaxes the moiré lattice into areas of energetically favorable stacking, creating a regime of triangular domains with alternating stacking of metal atoms aligned over chalcogen (MX), and chalcogens aligned over metal atoms (XM). Broken inversion symmetry in these domains leads to vertical polarization. Here, we explore the question of how this spatially varying polarization is influenced by and influences a proximal electrostatic environment. We show Scanning Tunneling Microscopy/Spectroscopy (STM/S) on graphene placed on top of marginally twisted WSe_2. In addition, using Kelvin Probe Force Microscopy (KPFM) we study how polarization depends on the substrate on which the marginally twisted layers are placed.

Merging Topography and Vibrations: STM-UHV-TERS Synergy for Low-Dimensional Materials

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Low-dimensional materials such as graphene and ultrathin oxide films have attracted significant attention in surface science due to their unique electronic, chemical, and mechanical properties, making them highly versatile for applications in nanotechnology, and catalysis. To probe these materials at atomic and molecular resolution, we employed an Ultrahigh vacuum scanning tunneling microscopy (UHV-STM) that provides sub-nanometer resolution imaging and pristine sample preparation along with tip-enhanced Raman spectroscopy (TERS) that was utilized to obtain vibrational fingerprints of these ultrathin oxide films, providing complementary chemical insights at the nanoscale.

Graphene has been employed as a substrate to grow Ni nanoclusters: at room temperature, nickel formed three-dimensional clusters on graphene, while at elevated temperatures, it intercalated beneath the layer to form a two-dimensional structure. We further explored ultrathin oxide films, specifically FeO and MgO, to investigate their nanoscale structures and catalytic properties. Well-ordered FeO islands exhibit distinct O-terminated and Fe-terminated edges, each hypothesized to exhibit different catalytic activities. To probe the specific reactivity of these edges, we employed a selective blocking strategy by depositing Pd and Pt, which preferentially bind to one edge type, thereby isolating the catalytic contributions of each termination. Comparative analysis of Fe-edge-blocked, O-edge-blocked, and edge-free FeO allows us to elucidate the mechanistic roles of these edges in catalytic reactions.

On Ag substrates, MgO formed both embedded and top-layer islands, along with Ag adatoms. By applying UHV-TERS, we distinguished their unique vibrational signatures, enabling chemical differentiation of the nanostructures. Together, this work highlights the complementary strengths of STM and TERS in unraveling the structure–reactivity relationships of low-dimensional materials, offering a foundation for the rational design of future nanoscale catalytic systems.

Understanding the Impact of Interfacial Co-Ions on Electric Double Layer Formation and Electrochemical Reactions

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Electrochemistry plays a central role in energy conversion, sustainable chemistry, and biomedicine. Electrochemical devices often hinge on chemical processes at charged electrode-electrolyte interfaces, where intermolecular forces cause electrolyte ions to be attracted or repelled from interfacial environments. Electrostatically, oppositely-charged counterions are attracted and like-charged co-ions are repelled, leading to charge separation that screens surfaces. Yet, this ion de-mixing also incurs substantial entropic penalties. Electric double layer formation describes how electrostatic and entropic forces balance to govern ion distributions and charge transfer at interfaces. While classical models for double layer formation predict co-ions are excluded from charged surfaces, we show that co-ions can play a defining role in electrocatalytic reactions under the high surface potentials inherent to many electrochemical systems. We reveal that co-ion identity has a significant influence on reactivity in both the hydrogen evolution reaction in aqueous solutions and the carbon dioxide reduction reaction in acetonitrile solutions. We utilize total electron yield X-ray absorption spectroscopy to show high surface potentials drive co-ion to accumulate at interfaces, contradicting expectations from classical theory. Further, we show co-ions can be designed with specific chemical functionalities to promote reactivity, such as acting as a hydroxide sink to buffer the interfacial environment. Overall, this study provides fundamental insight into how co-ions can play an important role in modulating reactions at charged interfaces.