Nanoscale Science and Technology
Room Ballroom A - Session NS-ThP

Nanoscale Science and Technology Poster Session

NS-ThP-1 Improving Mechanical Integrity in Wearable Solid-Carbon Microneedle Sensors, ***Nicolas Manning***[1], Commonwealth University of Pennsylvania - Lock Haven

Nanostructured carbon used as solid contact enables stable, calibration-free all-solid-state ion-selective electrodes (SC-ISEs) in miniaturized formats. It is typically coated on top of a metallic electrode, such as a microneedle, followed by an ion-selective membrane (ISM) coating. When this microneedle is inserted into artificial skin, the coatings do not always stay intact. Here we investigate an alternate approach by preparing self-supporting mesoporous carbon-based microneedles, which can be infiltrated and covered with the ISM. We hypothesize that this helps to maintain the ISM coating during insertion of the microneedle into skin. Silicone molds were prepared from steel microneedle arrays and then infiltrated with a resol containing colloidal silica as sacrificial template for the mesopores. After polymerization and carbonization, the resulting microneedle arrays were etched to remove the silica, introducing mesopores. Structural features were verified by scanning-electron microscopy. Future work will incorporate reference membranes and assess ion selectivity under physiological conditions, advancing SC-ISE microneedles for real-time on-skin or in vivo ion monitoring.

NS-ThP-2 Single-Molecule Spectro-Microscopic Visualization of Surface-Supported Configurational Flexibility and Intramolecular Transformations, ***Soumyajit Rajak***[2]*, Nan Jiang,* University of Illinois, Chicago

Understanding physicochemical transformations at surfaces with molecular-scale precision is essential for advancing nanoscale materials characterization and the rational design of functional interfaces for catalysis, molecular electronics, and optoelectronic devices. A major challenge in surface characterization is the direct identification of intermediates, adsorption geometries, and reaction products with simultaneous chemical specificity and sub-molecular spatial resolution, capabilities that are difficult to achieve with conventional ensemble-averaged techniques. Although scanning tunneling microscopy (STM) provides atomic-scale structural information, it often lacks definitive chemical sensitivity, particularly for nonplanar and conformationally flexible molecular systems. A single-molecule tip-enhanced Raman spectroscopy (TERS) methodology integrated with ultra-high vacuum (UHV) STM has been utilized to achieve correlative nanoscale structural and chemical characterization of thermally induced surface transformations and surface-dependent molecular arrangements. Coupling light with an atomically sharp plasmonic probe creates highly localized surface plasmons (LSPs), which allow the overcoming of the diffraction limit and confined enhancement of the Raman signals. As a model metal-organic interface, we investigate tetraphenyl tetrabenzoporphyrin adsorbed on Cu(100) and Cu(111), representative systems relevant to heterogeneous catalysis and organic electronic materials. Porphyrin derivatives are especially attractive for nanoscale studies because of their tunable electronic structure, metal-coordination functionality, and conformational flexibility arising from σ-bonded meso-substituents.Our measurements demonstrate that TERS provides chemically specific vibrational fingerprints of individual adsorbed molecules while simultaneously resolving symmetry variations and local conformational changes induced by molecule–substrate interactions at the sub-nanometer scale. Spatially resolved vibrational mapping enables discrimination between coexisting adsorption geometries and thermochemically transformed species that exhibit distinct chemical identities. The results further reveal how substrate interactions stabilize nonplanar conformations and alter molecular symmetry, establishing direct structure-property relationships at the single-molecule level.

NS-ThP-3 Intrinsic Stability of Rhodium Nanoclusters on HOPG: An Atomic-Scale Investigation of Heat Treatment and CO Adsorption, ***Charbel Tawny***, *Maxwell Gillum, Gallage KPA Ariyaratne, Mausumi Mahapatra,* Loyola University Chicago

Understanding structure-reactivity relationships in heterogeneous catalysis requires well-defined model systems that enable atomic-scale characterization. In this work, Rhodium (Rh) nanoclusters were deposited on Highly Oriented Pyrolytic Graphite (HOPG), an inert support, to investigate their nucleation, growth and changes in morphology under ultra-high vacuum (UHV) conditions. By systematically varying Rh coverage (0.09 ML to 0.6 ML), Scanning Tunneling Microscopy (STM) was used to resolve cluster size, morphology, and spatial distribution. Our experiments reveal the formation of highly dispersed Rh nanoclusters with a notably narrow size distribution; for instance, a 0.09 ML deposition produced particles with an average width of 1.74 ± 0.5 nm and height of 0.85 ± 0.1 nm. Crucially, these nanostructures exhibit exceptional thermal stability, maintaining their size and distribution even after annealing to elevated temperatures up to 850 K. Subsequent CO exposure at both 300 K and 500 K allowed for the visualization of surface interactions. While CO induced streaking was observed in STM images due to adsorbate mobility, the Rh clusters remained structurally stable without significant redispersion or morphological changes. This study establishes the robustness of Rh nanoclusters in response to various stimuli that would be present in an industrial reaction, such as high temperatures and gas exposure, further deepening our knowledge of surface catalysis.

NS-ThP-4 Characterization and Analysis of Rhodium Oxide Nanoparticles on HOPG Surface, ***Gallage KPA Ariyaratne***, *Maxwell Gillum,* Loyola University Chicago*; Charbel Tawny,* loyola University Chicago*; Mausumi Mahapatra,* Loyola University Chicago

This study investigates the characterization and analysis of rhodium oxide (RhO_x) nanoparticles formed on highly oriented pyrolytic graphite (HOPG), with the aim of understanding how oxygen influences nanoparticle stabilization and behavior on a weakly interacting support. HOPG serves as an ideal model surface for probing intrinsic nanoparticle properties in the absence of strong substrate interactions. Rh nanoparticles are vapor-deposited onto freshly cleaved HOPG under ultra-high vacuum conditions and subsequently oxidized at controlled temperatures (300–850 K) to generate RhO_x nanostructures. Scanning Tunneling Microscopy (STM) is employed to examine nanoparticle morphology, size distribution, and structural evolution as a function of temperature and Rh coverage. Oxidation at room temperature results in the formation of RhO_x nanoparticles with an apparent reduction in particle density and surface coverage relative to metallic Rh. At elevated temperatures, larger RhO_x nanoparticles are observed, with average widths of 9.14 nm. High temperatures like 850 K, result in the formation of triangular channels on HOPG surface, originating from step edges. These features are not due to direct structural failure of HOPG but rather arise from oxygen mediated anisotropic etching of the graphite surface. Oxygen can dissociate on RhO_x which then migrate onto the HOPG surface where the atomic oxygen react with uncoordinated carbon atoms at defect sites and step edges which lead to the removal of carbon atoms as CO/CO_2 and leads to anisotropic etching on surface. Post oxidation exposure to carbon monoxide (CO) is performed to evaluate redox reversibility and stability under reducing conditions, with the evolution of gaseous species such as CO_2, O_2, and CO observed, while the crack and particle size remains unchanged. In parallel, Density Functional Theory (DFT) calculations using (PBE-GGA) model RhO_x adsorption on graphite, identifying favorable configurations, and electronic properties with nanoparticle stability, reactivity, and catalytic performance on carbon supports.

NS-ThP-5 Spatiotemporal Defect Engineering of Charge Transport in TiO2 by Time-Resolved Atomic Force Microscopy, *Nuray Basaran, Mohammad Safikhani-Mahmoudi,* École de technologie supérieure, University of Quebec, Canada*; **Bugrahan Guner**,* Yale University*; Omur Dagdeviren,* École de technologie supérieure, University of Quebec, Canada

The performance of photocatalysts, sensors, and oxide-based devices is governed by how charge carriers migrate, recombine, and interact with defects at surfaces and interfaces. Titanium dioxide (TiO_2), a model photocatalyst, provides a versatile platform for exploring these dynamics. Recent advances in*time-resolved atomic force microscopy (TR-AFM)* now allow direct nanoscale mapping of carrier motion under realistic conditions, uncovering defect-controlled pathways that were previously inaccessible.

We establish findings from our recent studies to build a coherent picture of light-induced defect dynamics in TiO_2. In "thin" TiO_2films, it was shown that ultraviolet irradiation generates photoinduced surface oxygen vacancies (PI-SOVs) that shorten carrier migration time constants but raise activation barriers, indicating a trade-off between faster trapping and reduced mobility. Extending this framework,*we*revealed that PI-SOVs impact both fast and slow timescales, with spatially heterogeneous distributions leading to locally distinct transport regimes.*Moreover, we explored* surface chemistry by introducing methanol as a prototypical hole scavenger:

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methanol adsorption further reduced time constants and modified activation energies, demonstrating how molecular adsorbates tune vacancy-carrier interactions.

By bridging molecular adsorption, defect generation, and irradiation penetration, this body of work highlights spatiotemporal defect engineering as a promising strategy for controlling charge transport in oxides. TR-AFM emerges as a uniquely powerful platform for resolving these processes at the nanoscale, offering pathways to rationally design oxide-based systems with tunable photocatalytic efficiency, sensor responsiveness, and energy-conversion robustness.

NS-ThP-6 Ce-Doped TiO_2 Nanoparticles from Commercial P25 and Flame Spray Pyrolysis Synthesis Routes for Enhanced Visible-Light Photocatalysis, *Selda Topcu Sendogdular,* Stony Brook University, Turkey*;* ***Ilker Keseroglu****, Pelagia-Iren Gouma,* The Ohio State University

Ce-doped TiO_2 nanoparticles were synthesized by modifying commercial Degussa P25 and flame-made TiO_2 produced by flame spray pyrolysis (FSP), followed by thermal treatment at 500 °C. The effects of Ce doping on the structural, morphological, optical, and photocatalytic properties of TiO_2 were investigated for undoped and Ce-doped samples containing 5 and 40 wt% Ce.

X-ray diffraction (XRD) analysis showed that both P25 and FSP TiO_2 consisted primarily of anatase and rutile phases, while Ce doping suppressed the anatase-to-rutile transformation and promoted CeO_2 phase formation at higher Ce loading. Ce doping reduced the anatase crystallite size and altered the phase composition, with brookite contributions observed in CE5-P25 and CE5-TiO_2 samples. SEM and TEM analyses revealed morphological differences between P25 and FSP TiO_2 particles, where P25 exhibited irregular elongated and polygonal particles, while FSP-derived TiO_2 showed predominantly spherical particles. Ce doping decreased particle size to approximately 14–34 nm, whereas high Ce loading (40 wt%) resulted in particle agglomeration and cube-like Ce-rich structures. SAED and HRTEM analyses confirmed the coexistence of anatase and rutile phases and verified lattice fringes corresponding to anatase (101) and rutile (110) planes.

UV–Vis spectroscopy demonstrated enhanced visible-light absorption and a red shift in the absorption edge with increasing Ce content. The bandgap decreased from approximately 3.06 eV for pure TiO_2 to 2.48 eV for Ce-doped samples, indicating improved visible-light response. Photocatalytic performance was evaluated through methylene blue degradation under visible-light irradiation using a Xe lamp with AM 1.5G and a 400 nm cut-on filter. Among all samples, CE5-TiO_2 exhibited the highest photocatalytic activity, achieving approximately 90% methylene blue degradation under visible light.

The enhanced photocatalytic performance is attributed to reduced crystallite size, suppression of rutile phase growth, modified phase composition, and improved visible-light absorption induced by Ce doping. These results demonstrate that Ce modification effectively enhances the photocatalytic activity of both commercial P25 and flame-made TiO_2 for environmental remediation applications.

NS-ThP-7 Roll-to-Plate Nanoimprint Lithography for Fabrication of Biomimetic Structures, ***Daniela Topasna****, Juan Gonzalez, Sebastian Ziegler,* Virginia Military Institute

Nanoimprint Lithography (NIL) fabrication technique consists of transferring a pattern from a template by pressing it onto a resin coated substrate, yielding structures with nanometer resolution. The resin can be cured thermally or by exposure to UV radiation. This is a simple, low-cost and high-throughput technique, which has been used as an alternative to photolithography in semiconductor industry, optics and photonics, and biomedical field. NIL roll-to-plate method was used in this project to replicate microstructures of Cicada wings which are of interest due to their antibacterial properties. We report the results on the fabrication of these biomimetic structures and on their characterization by scanning electron microscopy.

NS-ThP-8 Nanoscale Surface and Interface Engineering of Asymmetric Electrode Screen Length for Advanced Nanoscale Ferroelectric Devices, ***Philip (Sanghyun) Lee****,* University of Kentucky*; Kent Price,* Morehead State University*; M. David Henry,* Sandia National Laboratories, USA

The continued scaling of ferroelectric tunnel junctions (FTJs) has placed unprecedented importance on understanding and controlling nanoscale surface and interface interactions within ultrathin HfO_2–based ferroelectrics. At thicknesses below 6 nm, the electronic structure, bonding environment, and screening behavior at metal/ferroelectric interfaces dominate the tunneling landscape, often more strongly than the bulk ferroelectric properties themselves. Conventional symmetric Metal-$Hf_{0.5}Zr_{0.5}O_2$-Metal (MFM) stacks such as TiN/HZO/TiN exhibit negligible tunneling electroresistance (TER) because their interfaces screen polarization charges in an identical manner, suppressing any barrier asymmetry. While inserting dielectric interlayers can restore asymmetry, these additional interfaces introduce variability, trap formation, and integration challenges.

This contribution presents a materials–driven strategy that leverages intrinsic nanoscale surface and interface asymmetry between dissimilar metal electrodes to enhance FTJ performance without modifying the ferroelectric layer. We focus on five CMOS compatible metals such as TiN, W, Ru, TaN, and Mo about possessing distinct electronic screening behavior, interfacial bonding characteristics, and surface chemistries with HZO. These differences affect how polarization-bound charges are compensated at the interface, reshaping the tunneling barrier.

To assess these nanoscale interfacial effects, multiple devices including Ta/HZO/TaN were developed and their nanoscale interfacial structures and chemistry were compared in agreement with theoretical research for MFM devices. This study incorporates realistic ferroelectric switching, nonlocal tunneling transport, and metal–specific screening behavior, enabling direct correlation between nanoscale interface physics and device–level performance. Surface and interface characteristics with multiple HZO thicknesses were quantified to confirm how interfacial screening, depolarization stability, and surface-induced barrier shaping collectively determine TER, read current, and write voltage.

Our results show that electrode pairs with different interfacial screening length create strong asymmetry in the tunneling barrier, enabling enhanced TER without the need for additional interlayers. Energy band analysis reveals how nanoscale surface interactions such as metal-oxygen bonding, interfacial dipole formation, and screening charge distribution directly affect the tunneling mechanism in opposite polarization states. Finally, we mapped optimal metal combinations that support low–voltage switching and stable ferroelectric behavior <6nm HZO for interface–engineered MFM devices.

NS-ThP-9 Time-Delayed Measurements of Heterogeneous Dynamic Data, ***Petro Maksymovych****,* Clemson University*; Sabine Neumayer,* Oak Ridge National Laboratory, USA

In neuromorphic and memory devices, accessible multistability is enabled by the dynamics of the constitutive materials rather than by their equilibrium structures alone. Hysteresis loops, oscillatory responses, and other time-dependent signatures reflect the multiplicity of accessible material states. Yet deciphering the underlying dynamics remains persistently elusive — in no small part because the dynamic information itself is treated qualitatively rather than as a quantitative observable.

I will present a systematic approach based on time-delayed embedding and dynamic mode decomposition that treats dynamic data as a structured object, extracting its nonlinearity, topology, and a predictive numerical model of the underlying process. Applied to resistive switching in memory oxide materials [1,2], nonlinearity alone can discriminate between specific microscopic mechanisms. In ferroelectrics, the same framework separates genuine switching from spurious hysteresis and detects the signatures of a multiwell potential [3,4]. Effective denoising strategies extend the approach to noisy nanoscale and device measurements without loss of physical interpretability.

Time-delayed methodologies provide a transparent and interpretable connection between hysteresis loops and physical mechanisms, complementing machine learning methods and enabling parameter-free comparison between modeling and experiments of driven dynamics. R

esearch sponsored in part by Division of Materials Science and Engineering, Basic Energy Sciences, Office of Science, US DOE at the Oak Ridge National Laboratory, and, at Clemson University by the State of South Carolina through funding for the Battelle Savannah River Alliance Workforce Development Program.

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NS-ThP-10 Chirality Retention in Aqueous Propylene Oxide Hydration: Chirality of the Transition State, ***Nisha Shukla***[1], Carnegie Mellon University, USA; *Marcus Yu,* University of Columbia; *Andrew Gellman,* Carnegie Mellon University, USA

The hydration kinetics of enantiomerically pure propylene oxide (PO) to chiralpropylene glycol (PG) in aqueous solution have been studied using FTIRwhile simultaneously monitoring the net chirality of the reaction mixture. The hydration reactionappears to be first-order in the PO concentration with a rate constant of 0.05 hr. Moreimportantly, the reaction is enantioselective; the product PG retains the chirality of the 2C carbonin PO with ~2:1 selectivity. The fact that there is some inversion of the chirality suggests thatthe dominant transition state is one in which the 2C-O bond in PO is cleaved, resulting in a closeto planar transition state capable of inversion during hydration. If the transition state involved1C-O cleavage it would retain the rigid chiral center of the PO reactant, preventing significantinversion.

NS-ThP-11 Understanding the Structural Orientation of Iron Tetraphenylporphyrin (Fe-TPP) on HOPG through Scanning Tunneling Microscopy for Electrocatalytic CO_2 Reduction, ***Hritvik Bhosale***, *Mausumi Mahapatra,* Loyola University Chicago

Homogeneous molecular catalysts provide precise control over the steric and electronic properties of active sites, enabling tunable catalytic activity and selectivity. However, these systems often suffer from limited stability, poor recyclability and reduced long-term durability under homogeneous operating conditions. Consequently, strategies that combine the tunability of molecular catalysts with the robustness of heterogeneous platforms have attracted considerable attention. Despite advances in catalyst heterogenization, developing structurally well-defined systems that bridge homogeneous and heterogeneous catalysis remains a challenge.

Porphyrin-based systems have emerged as attractive molecular platforms owing to their structural versatility, electronic tunability and catalytic relevance. Among them, iron porphyrins are particularly promising for electrocatalytic CO_2 reduction through successive electron-transfer processes that have demonstrated efficient, CO-selective and durable catalytic performance.

Understanding molecule-surface interactions at the nanoscale is essential for rational catalyst heterogenization. Scanning tunneling microscopy (STM), with submolecular and atomic-scale spatial resolution, provides a powerful platform for directly visualizing molecular arrangements, conformations, electronic structures and intermolecular interactions at surfaces. STM has proven especially effective for investigating the adsorption behavior and self-assembly of porphyrin systems on conductive substrates.

The present study investigates the adsorption behavior of iron tetraphenylporphyrin (FeTPP) on highly oriented pyrolytic graphite (HOPG) using STM as the primary investigative technique. By correlating molecular structure with surface organization, intermolecular interactions, and local electronic properties, this work aims to provide fundamental insights into molecule-surface interactions relevant to catalyst heterogenization and to establish structure–property relationships for the development of heterogenized iron porphyrin systems for efficient electrocatalytic CO_2 reduction.

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NS-ThP-12 Nano-Projectile SIMS: Guiding EUV Resists Fabrication Process with Nanoscale Compositional Insights, ***Christelle Guillermier***, Biennetechnology; *Michael J Eller,* University of Mississippi; *Stanislav V Verkhoturov, Richard Rickman,* Biennetechnology; *Serge Della Negra,* Universite Paris Saclay, France; *Emile A Schweikert,* Texas A&M and Biennetechnology

The semiconductor industry is rapidly adopting extreme ultraviolet (EUV) lithography to pattern features below 10 nm. However, there remains a critical need for methods capable of probing nanoscale compositional uniformity throughout the multi-step fabrication process. Secondary Ion Mass Spectrometry (SIMS) has long been a key analytical technique in semiconductor process control due to its high sensitivity and high-resolution depth profiling capabilities, but its lateral resolution is limited to ~50 nm, restricting its application to critical dimension analysis. In this work, we present results from the newly commercialized Nano projectile Secondary Ion Mass Spectrometry (NP-SIMS) instrument, the Orion MkII, which overcomes this limitation by examining surfaces with individual nano-projectiles. Each projectile samples an area of ~10–15 nm in diameter and ~10 nm in depth, enabling nanoscale inspection with lateral resolution that matches the requirements of advanced EUV photoresist characterization. We demonstrate the capabilities of NP SIMS for identifying material inhomogeneities that can lead to defects during resist fabrication and compromise pattern quality. More specifically, NP-SIMS enables examination of characteristic molecular species for homogeneity and co-localization with other resist components. The integration of a multi-anode detector further allows identification and characterization of sites containing multiple instances of the same analyte. Finally, NP-SIMS provides detailed chemical analysis of defect sites, which can significantly affect the resist performance. Altogether, NP-SIMS delivers essential insights to guide the optimization of EUV resist chemistry and processing conditions.

NS-ThP-14 Local Electronic and Transport Properties of Epitaxial Graphene on Sic(0001) Studied by Scanning Tunneling Microscopy and Spectroscopy, ***Marek Kolmer***, *Umamahesh Thupakula, Shen Chen, Yong Han,* Ames National Laboratory; *Michael C. Tringides,* Iowa State University

Despite long-standing efforts to understand the interface between epitaxial graphene and the Si-terminated silicon carbide (0001) substrate, the exact atomic-scale structure, its complex bonding configurations, and the resulting electronic properties of the first epitaxial graphene carbon layer (C_{buffer}) remain open problems. We will present how to control the local structure of the epitaxial graphene-SiC interface with a low-temperature scanning tunneling microscope (STM) [1]. We will show that the covalent bonds between C_{buffer} and the SiC substrate may be reversibly broken and restored using the polarity of the electric field from the STM tip, generating protrusions at the interface of slightly higher amplitude. This buried interface manipulation enabled us to pattern epitaxial graphene with lateral precision, reaching the scale of a single 1.8 nm unit cell of the graphene-SiC interface $(6\times6)_{SiC}$ moiré lattice. However, the STM manipulation experiments also provide direct evidence of silicon vacancies at the topmost reconstructed SiC(0001) layers [2]. Bias-voltage- and epitaxial graphene thickness-dependent characterization of the collective C_{buffer}-SiC interface showed that 'Si' vacancy sites exhibit stable, non-switching behavior under STM electric fields. Moreover, vacancies introduce localized electronic states below the Fermi level. Our experimental results directly elucidate the atomic-scale interface and the influence of atomic and bonding configurations on the local density of states for graphene of different thicknesses on SiC(0001). Finally, we will present the consequences of the local epitaxial graphene structure on electronic transport properties.

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NS-ThP-15 The Nature of Photodoping in van der Waals Heterostructures, ***Son Le***, Laboratory for Physical Sciences; *Thuc Mai, Maria Munoz, Riccardo Torsi, Angela Hight Walker, Curt Richter,* NIST; *Aubrey Hanbicki,* Laboratory of Physical Sciences; *Adam Friedman,* Laboratory for Physical Sciences

A unique photoinduced modulation doping is achieved via integration of common 2D materials and inexpensive light sources. Under applied electric field and incident light, the doping level of 2D materials heterostructures consisting of multiple dielectric layers can be precisely controlled and tuned *in situ*. This photodoping also offers local control of charge with submicron spatial resolution with lifetimes on the order of months to years. For 2D

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materials systems there is no current agreement on the exact mechanism underlying this effect, with studies pointing to charge generation and trapping in various layers/interfaces. In this work, we present photoinduced doping of van der Waals heterostructures with various compositions in order to pin-point the exact spatial location of the photoactive defects that responsible for the doping phenomena. Regardless of the mechanistic details, this photodoping effect yields high-quality reconfigurable devices in a variety of 2D material systems including graphene, TMDs, and 2D superconductors.

Reference

Son T. Le *et al., 2D Mater.* **12** 015006 (2025)

NS-ThP-16 Ternary Gold Nanoparticle-Corona-Neurotransmitter Plasmonic Complexes for Probing Resonant Electronic Coupling*, **Tefera Entele Tesema**, Kahmeria Smith,* Prairie View A&M University

Plasmonic gold nanoparticles generate localized electromagnetic fields under resonant excitation, making them powerful platforms for probing nanoscale metal–molecule interactions. Although the molecular corona is often treated as a passive stabilizing layer, its composition can regulate interfacial charge distribution, optical damping, adsorption geometry, and plasmon-mediated coupling. Here, we develop a ternary plasmonic complex consisting of a gold nanoparticle core, a plant-derived molecular corona, and neurotransmitter molecules as a model system for resonant electronic coupling at bioactive noble-metal interfaces, using surface-enhanced Raman scattering (SERS) as the primary readout.Purple sweet potato (Ipomoea batatas, PSP)-derived extract functions as a reducing/stabilizing medium and forms a molecular corona containing anthocyanins, phenolic acids, and related polyphenols. This corona is treated as an electronically active, chromophoric interface whose absorption can influence resonance conditions. Dopamine is used as an initial catecholamine model to probe how bioactive adsorbates perturb the corona-mediated optical and vibrational response.Preliminary UV–visible spectroscopy shows that extraction protocol, pH, and solvent environment influence the optical identity of the PSP extract and nanoparticle formation. Unpeeled PSP extracted in 0.05 M acetate buffer at pH 4.75 produces a wine-colored, colloidally stable AuNP suspension that remains visually stable for five days. In contrast, TFA extraction at pH ~3 preserves anthocyanin absorption near 522 nm but is associated with black precipitate during AuNP formation, consistent with uncontrolled nucleation or aggregation. These observations indicate that mildly acidic acetate conditions provide a more suitable window for controlled AuNP–corona assembly. Anthocyanin interconversion among flavylium, hemiketal, quinonoidal, and related forms provides a handle for tuning corona absorption relative to the AuNP plasmon and SERS excitation.The phenolic and catechol-like functionalities in the PSP corona overlap chemically with catecholamine neurotransmitters and may compete for or reorganize interfacial binding sites on gold. SERS will monitor these interactions through vibrational fingerprints that report adsorption geometry, orientation, and binding competition. Coupling corona electronic transitions, nanoparticle plasmon resonance, and laser excitation is expected to amplify neurotransmitter-sensitive interfacial signatures. This work provides a tractable model for signal transduction at biotic–abiotic interfaces and may inform plasmonic chemical sensing and bioactive nanoparticle design.

NS-ThP-17 Exciton-Polaritons in Metal-Organic Chalcogenolates: From UV to Visible*, **Deep Jariwala***[1], University of Pennsylvania

Exciton-polaritons (EPs), hybrid light–matter quasiparticles formed by strong coupling between excitons and confined photons, offer a route to engineer semiconductor optical response without chemical modification. Here, I present strong and ultrastrong coupling in metal-organic chalcogenolates (MOCs), layered van der Waals hybrid semiconductors that act as natural multi-quantum-well structures with strong excitons, large oscillator strengths, and high refractive indices. These properties make MOCs promising self-hybridized polaritonic materials from the ultraviolet (UV) to visible range.

I will first discuss silver phenylselenolate (AgSePh, mithrene), which has a direct optical bandgap of ~2.65 eV, exciton binding energy of ~400 meV, and refractive index of ~2.5. Mueller matrix ellipsometry reveals giant in-plane birefringence (~1.01) and three anisotropic exciton resonances, enabling polarization-dependent linear dichroism up to ~77% when coupled to an optical self-cavity. Thickness-controlled mithrene flakes on reflective substrates support self-hybridized EPs in the ultrastrong coupling regime, with normalized coupling g/Ex = 0.13–0.14 and Rabi splitting >650 meV, the largest reported for a non-organic semiconductor in the visible range.

I will then present self-hybridized EP photodetectors in mithrene, where thickness-tunable multimode polariton states enable sub-bandgap photodetection extending >130 nm (~0.55 eV) below the optical bandgap. Trap-assisted two-photon absorption sustains strong coupling under sub-bandgap excitation, addressing a key limitation for polaritonic light harvesting. The polariton dispersion yields ultrafast group velocities (~65 μm ps−1), extending effective exciton diffusion from hundreds of nanometers to several micrometers and producing a 2.38-fold enhancement in photo-to-dark current ratio.

Finally, I will extend these concepts to the UV using silver phenylthiolate (AgSPh, thiorene), a wider-bandgap MOC with a sharp excitonic resonance at 3.46 eV (~60 meV linewidth) and refractive index of ~2.1. In open and closed cavities, thiorene shows clear anticrossing with Rabi splittings of 488 and 512 meV, respectively, among the largest reported in the UV and 6–10× larger than conventional ZnO and GaN platforms. Together, these results establish MOCs as a versatile platform for polariton-enhanced optoelectronics.

[1] **JVST Highlighted Poster**

Author Index

Bold page numbers indicate presenter

— A —
Ariyaratne, Gallage KPA: NS-ThP-3, 1; NS-ThP-4, **1**
— B —
Basaran, Nuray: NS-ThP-5, 1
Bhosale, Hritvik: NS-ThP-11, **3**
— C —
Chen, Shen: NS-ThP-14, 3
— D —
Dagdeviren, Omur: NS-ThP-5, 1
Della Negra, Serge: NS-ThP-12, 3
— E —
Eller, Michael J: NS-ThP-12, 3
— F —
Friedman, Adam: NS-ThP-15, 3
— G —
Gellman, Andrew: NS-ThP-10, 3
Gillum, Maxwell: NS-ThP-3, 1; NS-ThP-4, 1
Gonzalez, Juan: NS-ThP-7, 2
Gouma, Pelagia-Iren: NS-ThP-6, 2
Guillermier, Christelle: NS-ThP-12, **3**
Guner, Bugrahan: NS-ThP-5, **1**
— H —
Han, Yong: NS-ThP-14, 3
Hanbicki, Aubrey: NS-ThP-15, 3
Henry, M. David: NS-ThP-8, 2
Hight Walker, Angela: NS-ThP-15, 3
— J —
Jariwala, Deep: NS-ThP-17, **4**
Jiang, Nan: NS-ThP-2, 1
— K —
Keseroglu, Ilker: NS-ThP-6, **2**
Kolmer, Marek: NS-ThP-14, **3**
— L —
Le, Son: NS-ThP-15, **3**
Lee, Philip (Sanghyun): NS-ThP-8, **2**
— M —
Mahapatra, Mausumi: NS-ThP-11, 3; NS-ThP-3, 1; NS-ThP-4, 1
Mai, Thuc: NS-ThP-15, 3
Maksymovych, Petro: NS-ThP-9, **2**
Manning, Nicolas: NS-ThP-1, **1**
Munoz, Maria: NS-ThP-15, 3
— N —
Neumayer, Sabine: NS-ThP-9, 2
— P —
Price, Kent: NS-ThP-8, 2
— R —
Rajak, Soumyajit: NS-ThP-2, **1**
Richter, Curt: NS-ThP-15, 3
Rickman, Richard: NS-ThP-12, 3
— S —
Safikhani-Mahmoudi, Mohammad: NS-ThP-5, 1
Schweikert, Emile A: NS-ThP-12, 3
Shukla, Nisha: NS-ThP-10, **3**
Smith, Kahmeria: NS-ThP-16, 4
— T —
Tawny, Charbel: NS-ThP-3, **1**; NS-ThP-4, 1
Tesema, Tefera Entele: NS-ThP-16, **4**
Thupakula, Umamahesh: NS-ThP-14, 3
Topasna, Daniela: NS-ThP-7, **2**
Topcu Sendogdular, Selda: NS-ThP-6, 2
Torsi, Riccardo: NS-ThP-15, 3
Tringides, Michael C.: NS-ThP-14, 3
— V —
Verkhoturov, Stanislav V: NS-ThP-12, 3
— Y —
Yu, Marcus: NS-ThP-10, 3
— Z —
Ziegler, Sebastian: NS-ThP-7, 2