Center for Quantum Materials Innovation and Education Excellence (CQ-MIEE)

Science and Technology of Emerging Materials Symposium 2025 (STEMS 2025)

November 15 – 16, 2025

Conference Abstracts

Session 1: Synthesis and Characterization of Quantum Materials

(Chair: Madhab Neupane)

Invited talk: Synthesis, Characterization and Application of Two-dimensional Materials

Eric M. Vogel, Georgia Institute of Technology

Two-dimensional materials such as graphene and transition metal dichalcogenides have attracted significant interest in recent years due to their properties. There is a large compositional space for 2-D materials which leads to their wide-ranging properties (metals, semiconductors, insulators). Some of their unique characteristics include potential for monolayer thickness control leading to ideal quantum wells and ultrathin diffusion/permeation barriers, lack of surface dangling bonds meaning heterostructures can be more easily formed, and flexibility with potential for being synthesized or transferred onto arbitrary substrates. This talk will cover the impact of the synthesis and structure of a wide variety of two- dimensional materials on their unique properties.

Invited talk: Probing and Controlling Topological Semimetals with In Situ Tunable Strain

Jiun-Haw Chu, University of Washington

Topological semimetals represent a class of three-dimensional quantum materials characterized by gapless electronic spectra and vanishing density of states near their band-crossing points. These features distinguish them from conventional metals and

insulators, offering a unique platform to explore novel electronic phenomena through external stimuli. In this talk, I demonstrate how in situ tunable strain serves as a powerful tool to both probe and manipulate the electronic states of topological semimetals. Focusing on ZrTe5 and Ta2NiSe5, I highlight two distinct strain-driven mechanisms. In ZrTe5, symmetry-preserving uniaxial strain induces a topological phase transition, enabling precise control over the negative longitudinal magnetoresistance—a unique feature associated with its Dirac semimetal phase. In Ta2NiSe5, symmetry-breaking shear strain directly couples to an excitonic phase transition, where electron-hole pair condensation drives the opening of a gap at Dirac points. These results illustrate how engineered strain can selectively modify electronic interactions and topological order, advancing strategies for manipulating novel phases in quantum materials.

Electronic structure of a rare Earth based nodal line semimetal candidate LnSbTe

Nathan Valadez, University of Central Florida; Milo Sprague, University of Central Florida; Iftakhar Bin Elius, University of Central Florida; Dante James, University of Central Florida; Tetiana Romanova, Polish Academy of Sciences; Sami Elgalal, Polish Academy of Sciences; Grzegorz Chajewski, Polish Academy of Sciences; Florie Mesple, University of Washington; Ellis Thompson, University of Washington; Keng Tou Chu, University of Washington; Matthew Yankowitz, University of Washington; Andrzej Ptok, Polish Academy of Sciences; Dariusz Kaczorowski, Polish Academy of Sciences; Madhab Neupane, University of Central Florida

Lanthanide-based LnSbTe materials provide a platform to study the interplay between magnetism, spin–orbit coupling (SOC), and topological states, driven by the presence of rare-earth 4f orbitals and nonsymmorphic crystalline symmetry.These compounds crystallize in a tetragonal structure consisting of a square Sb lattice sandwiched between Ln–Te planes, hosting rich electronic and magnetic behavior. Across the LnSbTe family, angle-resolved photoemission spectroscopy (ARPES) measurements reveal a characteristic diamond-shaped Fermi surface, a topological state located at the X point, and a nodal line along multiple high-symmetry directions. Low-temperature bulk measurements indicate magnetic transitions from paramagnetic to antiferromagnetic order, with transition temperatures varying by lanthanide element. In this study, we present a comparative investigation of several LnSbTe members, combining ARPES, low-temperature transport, and density-functional theory (DFT) calculations to explore the influence of SOC on the electronic band structure and the evolution of magnetic and topological properties within this material family.

Investigation of Chiral Phonons in Breathing Kagome Lattice Quantum Material Nb3TeCl7

Dylan A. Jeff, University of Central Florida; Tharindu Fernando, University of Washington; Jonathan DeStefano, University of Washington; Nelson Alvarez, University of Central Florida; Madhab Neupane, University of Central Florida; Jiun-Haw Chu, University of Washington; Saiful I. Khondaker, University of Central Florida

Nb3TeCl7 is a quantum material that features a breathing kagome lattice, contributing to the formation of topologically flat electronic bands and the presence of broken spatial inversion symmetry. Due to this broken symmetry, Nb3TeCl7 is a prime candidate for the observation of chiral phonons, defined as a collective oscillation of circularly polarizable phonons that carry pseudo-angular momentum. This momentum allows them to interact with other particles, such as electrons or photons, and actively influence their respective spin or the handedness of their circular polarizations via interaction. In this study, we utilize linearly and circularly polarized Raman spectroscopy to investigate the Raman-active phonon modes of exfoliated Nb3TeCl7 in search of chiral phonons. Our experiments resolve the fundamental irreducible representations of the phonon modes according to the linear polarization angle dependence of their corresponding Raman peak intensities, which are fitted utilizing the Raman selection rules of the D3d crystal system. Helically resolved Raman spectroscopy reveals that many of the phonon modes flip the helicity of the incident light upon scattering, evidence of the transfer of angular momentum and a telltale mark of chiral phonons.

Session 2: Calculation, Modelling and Characterization of Quantum Materails (Chair: Rongying Jin)

Invited talk: AI-Driven First-Principles Modeling of Moiré Superlattices

Ting Cao, University of Washington

Recent advances in twisted and layered two-dimensional materials have enabled unprecedented control over emergent quantum phases, including correlated and topological states. In this talk, I present our theoretical and computational efforts to understand and predict these phenomena through physics-aware artificial intelligence. We begin by demonstrating how deep neural networks trained on first-principles data can efficiently model moiré structural reconstruction in transition metal dichalcogenide superlattices. Going beyond the capacity of direct first-principles calculations, our machine-learning enabled workflow discovers salient structural features and key topological characters controlled by twist angles, layer composition, and other tuning knobs. This knowledge can be used to predict new forms of moiré potential and moiré topology, which enable the study of novel excited states.

Van der Waals quantum matter – systems composed of natural or artificially stacked two-dimensional layered materials – is extremely sensitive to the many-body interactions between its constituents.

Paulo Eduardo de Faria Junior, University of Central Florida

In particular, the suitable combination of layered materials is a highly efficient approach for studying emergent quantum phenomena and correlated phases in van der Waals heterostructures. In this talk, I will discuss important signatures of emergent spin and orbital textures in van der Waals matter focusing on three distinct scenarios: (i) the proximity-enhanced valley Zeeman splitting in WS2/graphene systems[1]; (ii) the emergence of purely radial Rashba spin textures in twisted homobilayers and hetero-multilayers of graphene and WSe2[2]; and (iii) the underlying physical mechanism of spin-polarized hole accumulation in vertical tunnel junctions of InSe/hBN[3].

[1] Faria Junior, Naimer, McCreary, Jonker, Finley, Crooker, Fabian, Stier, 2D Materials 10, 034002 (2023).

[2] Frank, Faria Junior*, Zollner, Fabian, Physical Review B (Letter, Editors' Suggestion) 109, L241403 (2024).

[3] Pasquale, Faria Junior, Feng, Collette, Watanabe, Taniguchi, Fabian, Kis, Nature Materials 24, 212 (2025).

Electrical and nonlinear optical properties in monolayer 2D kagome material Nb_3TeCl_7

Israel Herrera, Mrinmoy Roy, Tharindu Fernando, Dylan Jeff, Shuva Roy, Dr. Yannick Salamin, Dr. Saiful Khondaker, Dr. Ting Cao, Dr. Andrea Blanco Redondo, University of Washington, University of Central Florida, National Science Foundation, Partnerships for Research and Eduication in Materials (PREM)

Nb_3TeCl_7 is an emerging 2D material that is attracting significant interest due to its unique breathing Kagome structure, direct band gap, and potential applications areas such as photocatalytic water splitting, telecommunications and quantum technologies.Its potentially strong nonlinear response could enable enhanced performance in nonlinear waveguides, leading to lower power requirements and more compact devices architectures. However, the electronic and optical properties of Nb_3TeCl_7 are still not fully understood. In this project, we investigate a new approach to control Nb_3TeCl_7's electronic band structure and explore the impact on its nonlinear optical response. In addition, we propose an experimental method to characterize its third-order nonlinear optical properties.

Our computational work focused on using Density Functional Theory (DFT) to explore the electronic and structural properties of the material, while paying particular attention to the tunability of its bandgap via electron self-repulsion, a mechanism that has yet to be investigated experimentally. For the optical analysis we solved the Nonlinear Schrodinger Equation (NLSE) using the split-step Fourier method to simulate the propagation of the optical pulse under group-velocity dispersion and Kerr nonlinearity. This approach facilitates the calibration of what nonlinear response as well as the effective mode area that is required in order to achieve soliton formation, along with other nonlinear optical properties such as the nonlinear refractive index. The simulations reveal enhanced nonlinearities in 2D material-integrated waveguides compared to conventional waveguide-only cases, creating an incentive for advanced photonic devices for telecommunications, supercontinuum generation, and optical sensing. Our experimental work aims at quantifying the strength of the nonlinear optical effects in the monolayer 2D kagome material Nb_3TeCl_7. As a first step, we have performed measurements of selfphase modulation (SPM)-induced spectral broadening in bare silicon nitride waveguides as a function of input power. These measurements serve as a calibration reference and as a means to validate our experimental setup using well-understood materials. We are now in the process of transferring 2D materials (starting with MoS2 and followed by Nb_3TeCl_7) onto the silicon nitride waveguides. Subsequent measurements of the SPM-induced broadening in the hybrid waveguides, silicon nitride waveguides covered with 2D materials, that will allow us to extract the nonlinear properties of the 2D materials.

Epitaxial Growth and Structural Characterization of Bi_2Te_3 Thin Films on GaAs(100) by Molecular Beam Epitaxy

Nia Suitt, Himanshu Sheokand, Madhab Neupane**,** University of Central Florida

Bismuth telluride (Bi_2Te_3), a prototypical topological insulator has attracted significant attention due to its layered crystal structure and tunable electronic properties. However, the growth of high-quality Bi_2Te_3 thin films remains challenging because of the narrow stoichiometric window and strong dependence on substrate orientation and growth kinetics. In this work, we report the epitaxial growth of Bi_2Te_3 thin films by molecular beam epitaxy (MBE) on GaAs(100) substrates under ultra-high-vacuum conditions. A Te-rich flux ratio was maintained to suppress Te desorption and ensure stoichiometric film formation. The evolution of in situ reflection high-energy electron diffraction (RHEED) patterns revealed a transition from streaky to well-defined (1×1) reconstructions, confirming two-dimensional layer-by-layer growth. X-ray diffraction (XRD) measurements were performed to confirm the crystallinity and c-axis orientation of the grown films, while energy-dispersive X-ray spectroscopy (EDS) verified the expected Bi_2Te_3 stoichiometry through both atomic and weight composition analysis. These results highlight the importance of flux optimization and substrate orientation in achieving high-quality Bi_2Te_3 epitaxy, paving the way for device-scale studies of topological and thermoelectric phenomena.

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Lattice dynamics of quantum material PdPS3 investigated via polarized Raman spectroscopy

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$PdPS_3$, a member of the metal phosphorus trichalcogenide (MPX_3, X = S, Se) family, has recently emerged as a promising quantum material. The monolayer form of $PdPS_3$ is predicted to host multiple Dirac cones and exhibit topological magnetism, while its bulk counterpart displays multiple node-like electronic features near the Fermi level. In addition to its intriguing electronic and magnetic properties, $PdPS_3$ holds potential for catalytic and energy conversion applications. In this work, we investigate of the Raman-active phonon modes of mechanically exfoliated bulk $PdPS_3$ for the first time using excitation-dependent, thickness-dependent, and linearly polarized Raman spectroscopy. We track how the characteristic Raman spectrum evolves with layer number and how different excitation wavelengths influence the number and intensity of observable modes. Furthermore, our linearly polarized Raman measurements resolve the irreducible representations of the vibrational modes, providing detailed insights into the symmetry and lattice dynamics of $PdPS_3$. Our results establish a foundational understanding of the vibrational properties and Raman response of $PdPS_3$, providing essential benchmarks for future studies on its few-layer and monolayer forms in quantum material–based devices and energy conversion technologies.

Session 3: Emerging Materials for Energy and Electronics

(Chair: Titel Jurca)

Invited Talk: Conductive ruthenium oxide films with surface-orientation control as experimental models for oxygen evolution reaction studies

Dhananjay Kumar Department of Mechanical Engineering North Carolina A&T State University

This presentation reports on a study of ruthenium oxide (RuO2) films from the perspectives of synthesis, structure-property connection, and electrocatalytic properties. The goal of this study was to understand the oxygen evolution reaction (OER) mechanism on metal oxides by aligning the synthesis, electrochemistry, in-situ spectroscopy, and first-principles modeling toward fundamental studies. RuO2 is one of the well-known OER electrodes. However, understanding their OER mechanism has not been straightforward, as material variation affected the characterization outcomes. We have utilized a pulsed laser deposition method to grow RuO2 films with controlled thickness, orientation, and crystallinity. Transport and electrocatalytic measurements show that the conductivity, nature of charge carriers, and electrochemistry are strongly dependent on the films' orientations. Select RuO2 films were studied using electrochemical atomic force microscopy and non-linear spectroscopy. The surface symmetry of the RuO2 film was found to depend on applied potential. This observation was rationalized through surface water polarization and dissociation on RuO2, a picture that was verified via the first-principles modeling of the dehydrogenation of water. In reference to water splitting by a photocatalyst, we propose how an enhancement in the photocatalytic performance of titanium oxide (TiO2) can be achieved by forming a TiO2-RuO2 heterostructure junction. In a TiO2-RuO2 heterostructure junction, the recombination rate of the photo-generated charge carriers in the TiO2 layer is deterred by the transfer of electrons from the conduction band of the TiO_2 layer to the RuO_2 layer, which is promoted by the higher work function of RuO_2 than that of TiO_2.

Invited Talk: Nanocarbon Metal Composites with Increased Electrical Conductivity and Transmittance to Light

Lourdes Salamanca-Riba, Xiaoxiao Ge, Chris Klingshirn, Romaine Isaacs, Madeline Morales, Manfred Wuttig, Oded Rabin, Karen Gaskell; University of Maryland Daniel Cole, Chris Shumeyko, ARL Aberdeen Balu Balachandran, Argonne National Laboratory

Nanocarbon metal composites are desirable to take advantage of the excellent charge carrier mobility, high thermal conductivity and strength of carbon nanostructures, such as graphene and carbon nanotubes (CNT), and the high charge carrier concentration in metals. The composites are expected to have improved properties that make them unique candidates in applications such as high power transmission lines, interconnects, heat exchangers, motors, photovoltaic cells and transparent electrodes, among others. However, graphene and CNT are costly and difficult to make in large quantities. We use a process to synthesize graphitic nanostructures in metals by the application of a DC current to liquid metal containing particles of activated carbon. The process, called electrocharging assisted process, generates a region of very high current density which transforms the activated carbon particles from amorphous to crystalline graphitic nanoribbons. Upon solidification of the metal the nanoribbons self-assemble with an epitaxial relation with the metal. We have used Al 1350 and activated carbon particles of ~100 nm and obtained samples with global electrical conductivities more than 5% higher than the parent alloy as well as enhanced local stiffness, measured by nanoindentation. The conductivity enhancement is correlated with increasing crystallite size and concentration of the produced graphitic nanostructures. We have also deposited films of nanocarbon copper by e-beam deposition and pulsed laser deposition that show increased transmittance to light and increased oxidation resistance compared to pure copper films of the same thickness. These films could be used in transparent electrodes or interconnects. The electrocharging assisted process is universal and scalable to large scale manufacturing.

Electrocatalytic Ammonia Synthesis from Nitrate on Nickel Phosphide Nanocrystals

Melody Fernandez, University of Central Florida; Emily Nishiwaki, University of Washington; Sierra Goode, Trinity University; Thomas Egan, University of Central Florida; Brandi Cossairt, University of Washington; Xiaofeng Feng, University of Central Florida

Ammonia (NH_3), a critical component of fertilizers, is mainly produced via the energy-intensive Haber-Bosch process, while the widespread use of nitrogen fertilizers has led

to nitrate (NO_3^-) contamination of groundwater. Electrochemical reduction of nitrate to ammonia offers a promising strategy for both groundwater denitrification and sustainable ammonia synthesis. The development of such a process requires electrocatalysts with high activity and high selectivity toward NH_3 over competing products such as nitrite, across a range of pH conditions. In this work, we investigated nickel phosphide (Ni_2P) nanocrystals as potential electrocatalysts for the nitrate reduction reaction (NO3RR). We synthesized Ni_2P nanocrystals and characterized their morphology and composition using transmission electron microscopy (TEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The Ni_2P nanocrystals were deposited onto carbon paper electrodes and evaluated for NO3RR using linear sweep voltammetry and constant potential electrolysis to quantify the activity and selectivity at various potentials. The electrocatalytic performance of Ni_2P nanocrystals was further studied under acidic, neutral, and alkaline conditions to investigate the effects of electrolyte pH on NO3RR activity and selectivity, aiming to design broad pH-range electrocatalysts for efficient and versatile nitrate recycling.

Bow Tie Antenna Coupled with a Lead-Graphene Josephson Junction for Potential Millimeter-Wave Detection

Emily Frederick, University of Central Florida; Swastik Ballav, University of Central Florida; David Castro, University of Central Florida; Robert Peale, Truventic and University of Central Florida; Masahiro Ishigami, University of Central Florida

Monolayer graphene, with its tunable energy gap and unique electronic properties, is a promising material to integrate with lead-based Josephson junctions for high-sensitivity mm-wave detection. Lead, with a transition temperature of ~7 K, is a suitable superconductor in the device design. By creating 2D material stacks and employing a bowtie antenna geometry, the goal is to realize a video-mode detector operating in the mm-wave regime. Video-mode detection is a unique characteristic of a Josephson junction where Shapiro steps, created by an external radio frequency, cause a change in the critical current through the junction. The measured devices exhibit temperature- and bias-dependent I–V characteristics. These results establish a foundation for optimizing a graphene-based Josephson junction device toward sensitive mm-wave detection applications. In this work, the fabrication and characterization of lead–graphene Josephson junctions measured in an optical cryostat are presented, with potential future integration into mm-wave detection.

Session 5: Growth and electronic/optical properties of QMs/ Emerging Materials for Photonics and Electronics

(Chair: Andrea Blanco Redondo)

Invited Talk: Hidden anomalies in topological semimetal $PtBi_2$

Rongying Jin

SmartState Center for Experimental Nanoscale Physics, Department of Physics and Astronomy, University of South Carolina

The discovery of topological properties in quantum materials has generated a new subfield, namely topological physics, which is to study the microscopic geometries and symmetries that lead to particular phenomena. The complexity can be induced by broken crystallographic and/or time-reversal symmetry. The broken crystallographic symmetry results in the noncentrosymmetry (NCS) of a material, while broken time-reversal (TR) symmetry can result from the intrinsic magnetism or the external magnetic field. Second harmonic generation (SHG) is a nonlinear optical response that is sensitive to NCS and TR symmetry breaking. I will discuss our SHG investigation on Weyl semimetal $PtBi_2$ with NCS. Combined with single crystal x-ray diffraction refinement and magnetic susceptibility measurements, the variation of the SHG intensity with temperature may be explained in terms of the unique symmetry of $PtBi_2$.

Epitaxial growth of altermagnetic α-MnTe on GaAs(111)B substrate via molecular beam epitaxy.

Himanshu Sheokand, University of Central Florida; Madhab Neupane, University of Central Florida

The altermagnetic materials has emerged as a model system for studying spin-split electronic structures, yet controlled epitaxial growth on technologically relevant substrates remains challenging. Among the known candidates, MnTe stands out as a prominent altermagnetic material owing to its layered structure and high Néel temperature. Here, we report the molecular beam epitaxy (MBE) growth of high-quality α-MnTe thin films on GaAs(111)B substrates and provide a comprehensive analysis of the growth evolution and structural properties. Real-time reflection high-energy electron diffraction (RHEED) reveals a transition from three-dimensional island nucleation to streaky two-dimensional patterns, indicating the development of smooth, epitaxial layers despite the large lattice mismatch. Raman spectroscopy confirms the formation of the hexagonal NiAs-type phase through the observation of the characteristic phonon modes at 121 cm^{-1} and 140 cm^{-1}. X-ray diffraction measurements verify single-phase (0001) orientation, while scanning electron microscopy, energy-dispersive X-ray spectroscopy, and atomic force microscopy demonstrate uniform morphology, near-stoichiometric Mn:Te composition, and nanometer-scale surface roughness. These results establish a reliable growth protocol for α-MnTe on GaAs(111)B and provide a foundational platform for exploring strain-engineered altermagnetism and spin-dependent phenomena in epitaxial MnTe heterostructures. Acknowledgement: M. N. is supported by the US

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Electronic structure of charge density wave materials

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Charge density wave (CDW) phenomena in low-dimensional rare-earth chalcogenides have garnered considerable attention due to their strong coupling between lattice, charge, and magnetic degrees of freedom. Among this family, EuTe4, characterized by multiple Te square-net layers interleaved with a single Eu-Te layer, provides an ideal platform to explore the interplay between CDW order and localized 4f electron magnetism. In this work, first-principles density functional theory (DFT) calculations were employed to examine the electronic band structure modifications induced by the CDW modulation. Angle-resolved photoemission spectroscopy (ARPES) measurements revealed the opening of a CDW gap at the Fermi level and additional hybridization-driven gap features at higher binding energies. The low-lying CDW gap exhibits pronounced anisotropy, reaching its maximum along the Γ–Y high-symmetry direction and a minimum along Γ–X. Furthermore, low-temperature heat-capacity measurements performed under varying magnetic fields near the Néel temperature (Tn~6.9 K) enabled the construction of the magnetic phase diagram of EuTe4. These results provide comprehensive insight into the momentum-dependent Fermi-surface-nesting–driven CDW order and its coexistence with magnetic correlations in this layered rare-earth telluride.

Modifying Magnetic Order in Kagome Using Strain

Edward Perez, University of Central Florida; Sarah Edwards, Jonathan DeStefano; Dr. Jiun-Haw Chu, University of Washington

We investigate whether shear strain can tune the magnetic transition of the kagome metal $TbMn_6Sn_6$, a member of the R166 family exhibiting ferrimagnetic-to-ferromagnetic spin reorientation near 309 K. While prior studies have applied uniaxial or biaxial strain within the a–b plane, our work introduces a novel approach that applies shear strain along the

c-axis using a piezoelectric actuator (lead zirconate titanate, PZT). This configuration enables rotational symmetry breaking that directly couples lattice distortion to the magnetic order, revealing a new mechanism for tuning kagome magnetism.

A custom-built shear strain device sandwiches a polished $TbMn_6Sn_6$ crystal between two titanium shells layered with Stylcast epoxy. The titanium shells are mechanically coupled to PZT stacks, such that an applied DC voltage produces opposing displacements, shearing the sample along the c-axis. The strain magnitude scales linearly with applied voltage, with a measured effect of approximately 0.1 K shift in the magnetic transition temperature per 10 V.

Electrical transport measurements were performed using a four-probe configuration to minimize geometric and contact resistances from defects. Resistivity (ρ) was recorded as a function of temperature under controlled voltage bias using a Physical Property Measurement Environment (PPME). The derivative dρ/dT vs. T reveals a distinct peak associated with the magnetic transition. As the applied voltage increases from 10 V to 100 V, the transition peak systematically shifts toward lower temperatures, demonstrating a continuous, reversible strain-tuning effect. Fitting the peak positions yields a linear relationship between transition temperature (TSR) and applied voltage, confirming that shear strain effectively modulates the spin reorientation transition.

These results establish that shear strain, unlike traditional uniaxial strain, breaks rotational symmetries critical to kagome magnetism, offering a new axis for controlling spin–lattice coupling. This method expands the experimental toolkit for exploring magnetoelastic phenomena in frustrated systems. Future work will explore dynamics applying AC voltages to probe frequency-dependent magnetoelastic responses and potential coupling to magnetic field.

Spin-photon Defect Centers in Silicon for Scalable Quantum Technologies

Md Sakibul Islam, Kuldeep Singh, Nitesh Singh, Wayesh Qarony, University of Central Florida

Solid-state material platforms have been instrumental in realizing spin-based qubits with long optical and spin coherence, offering a pathway toward scalable quantum technologies, including quantum processors, quantum memories, and quantum communication networks. Among these, atomic defect-based color centers such as nitrogen vacancy (NV) and silicon vacancy (SiV) center in diamond, divacancies in SiC, quantum dots in III-V semiconductors, and defects in two-dimensional materials such as hexagonal boron nitride (hBN), have demonstrated remarkable progress in spin-photon interface, single photon generation and quantum sensing. However, each of these system faces intrinsic challenges that limit scalability. Diamond and SiC centers emit outside the telecom band and require complex heterogeneous integration, while quantum dots suffer from spectral inhomogeneity and device-to-device variation. To date, no single material platform has simultaneously met the requirements for quantum processing, quantum storage, and quantum networking within a fully CMOS- compatible framework.

Recent breakthroughs in silicon-based color centers have opened a new frontier by combining telecom band emission, long spin coherence, and native integration with silicon photonics. In particular, carbon-related defects in isotopically purified silicon such as G- and T- centers have shown promising characteristics as spin-photon qubits. The T-center, for example, has enabled long-lived spin-photon entanglement and demonstration of a three-qubit register, firmly establishing silicon as a credible host for scalable quantum technologies. Building on this progress, we recently demonstrated the femtosecond-laser-assisted generation of a novel isolated Ci center in silicon, which emits at ~ 1452 nm, within a low-loss telecom band, and exhibits a spin-triplet ground state suitable for spin-photon interface.

In this work, we present the monolithic integration of Ci center with a silicon nanophotonic cavity to enhance quantum light emission efficiency and photon indistinguishability through strong light-matter interaction. We design, simulate, and fabricate nanobeam cavities with high-quality factors exceeding 10^5 and mode volume below 0.6 (λ/n)3, enabling Purcell enhanced emission and life-time reduction. The deterministic "write/erase" placements of Ci center at the antinodes of the cavity is achieved using femtosecond-laser pulses with in-situ feedback ensuring sub-micron precision and reproducibility. The integrated devices are characterized through on-chip quantum measurements, including Hong-Ou-Mandel (HOM) experiments using off-chip superconducting nanowire detector, demonstrating photon indistinguishability.

This work establishes a fully CMOS-compatible silicon quantum photonic platform that unites nanophotonic design, simulation, fabrication, deterministic emitter creation, high-coherence spin-control, and integrated detection, representing a critical step toward large-scale, telecom band quantum processors, quantum memories and quantum networks.

Session 6: New Phenomena, Surfaces and Reactions in Emerging Materials (Chair: Parag Banerjee)

Invited Talk: What we cannot measure, we cannot understand: Bridging the gap with electron microscopy

Juan Carlos Idrobo, University of Washington and Pacific Northwest National Laboratory

Recent advances in monochromated, aberration-corrected, and cryogenic scanning transmission electron microscopy (STEM) are redefining our ability to probe emergent phenomena in quantum and energy materials at nanometer and atomic scales. By combining high-energy-resolution spectroscopy and imaging under in-situ electrical bias, these instruments now enable direct observation of charge-neutral transport and magnetic ordering in materials. In this presentation, I will discuss how we employ electron energy-loss spectroscopy (EELS), electron magnetic chiral dichroism (EMCD), and four-dimensional STEM (4D-STEM) to reveal the interplay between angular-momentum transport and magnetic ordering with lattice structure. I will conclude by outlining both the promise and the current experimental challenges in achieving truly quantitative, multimodal characterization of the aforementioned physical phenomena at the atomic scale. [1]

1. This work was partially supported by the U.S. Department of Energy (DOE), Office of Science (SC), Basic Energy Sciences, Material Sciences and Engineering Division, Electron and Scanning Probe Microcopies Program, FWP 83244, and by the U.S. National Science Foundation through the UW Molecular Engineering Materials Center (MEM-C), a Materials Research Science and Engineering Center (DMR-2308979). Some of the STEM experiments were supported by the Center for Nanophase Materials Sciences, which is a Department of Energy Office of Science User Facility, and conducted, in part, using instrumentation within ORNL's Materials Characterization Core provided by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

Invited Talk:Time-domain optical control of molecular and material dynamics

Tom Hopper, University of Central Florida

Since the advent of femtochemistry, researchers have sought to both monitor and manipulate quantum dynamics at the intrinsic length and time scales of atoms, electrons, and bonds. Two-pulse pump–probe experiments have long been the workhorse for these efforts, providing ultrafast snapshots of processes launched by optical excitation. In this talk, I will discuss how three-pulse pump–control–probe schemes allow us to direct the evolution of excited states in real time, thereby revealing the underlying energy landscape. I will highlight two directions: (i) semiconductor nanocrystals for optoelectronics, where optical probes track the interplay of electrons, lattice vibrations, and defects; and (ii) diatomic gas-phase molecules, where hard X-ray scattering enables spatiotemporal imaging of wavepacket shaping by coherent control. Together, these studies move beyond passive observation toward active control of the coupled electronic and structural dynamics that govern function in condensed phases.

Designer Catalyst Surfaces on Black Phosphorus

Hailey Akins, University of Washington; Andrei Draguicevic, University of Washington; Lauren Peck, University of Washington; Alexandra Velian, University of Washington.

Black phosphorus (bP), a layered 2-dimensional allotrope of phosphorus, exhibits a tunable layer- dependent bandgap and has emerged as a next generation Van der Waals material with remarkable electronic properties. Unlike other Van der Wals materials, the bP basal exhibits remarkable reactivity due to a network of localized electron lone pairs making it ideal for the installation of metallic sites with distinct functionalities. However, synthetic methods with which to precisely tune the identity and properties of these sites are scarce. By leveraging bP as a material analog to molecular phosphines, surface complexity ranging from atomically precise organometallic fragments to dispersed nanoscale structure can be realized. In this work, facile, solvothermal synthetic techniques are presented to install metallic sites with potential and demonstrated catalytic applications. Diffuse reflectance infrared spectroscopy is used to provide insights on the coordination environment of discrete, chemisorbed organometallic fragments with various potential functionalities.1 Additionally, sequential functionalization of bP with o-quinone precursors allows for the stabilization of multiple, distinct metal environments on the nanosheets. To probe the relevance such sites to electrocatalysis, group VI metal carbonyls were explored for their hydrogen evolution activity, demonstrating improved overpotentials relative to non-modified bP. Furthermore, treatment of nanosheets with chlorobis (cyclooctene)rhodium dimer results in dispersed nanoscale structures active for a variety of thermochemical hydrogenations. Work is ongoing to characterize the chemical identity of these structures. The functionalization of the bP surface demonstrates unique catalytic possibles and provides an avenue with which to gain fundamental insights into the role of bP as a catalytic support.

(1) Mitra, K. L. W.; Riehs, M.; Draguicevic, A.; Swann, W. A.; Li, C. W.; Velian, A. Angewandte Chemie International Edition 2023, 62 (49), e202311575.

Atom Economical Synthesis of Zinc Acetylacetonate Complexes

Justin Moore, University of Central Florida; Titel Jurca, University of Central Florida

Currently, diethyl zinc (DEZ) is used extensively as a precursor in atomic layer deposition (ALD) for the growth of zinc oxide (ZnO) and related films due to its high reactivity and volatility. However, it is extremely pyrophoric and requires specialized equipment to be handled safely. Zinc acetylacetonate (Zn-acac) complexes have shown some promise as alternative air stable, thermally robust precursors with tunable volatility. However, their synthesis remains limited, with metathesis reactions being the most common route and generating stoichiometric amounts of salt waste.

Inspired by parallel atomic layer etching (ALE) studies, which are functionally the reverse of ALD, we report the facile atom-economical solvothermal synthesis for a variety of Zn-acac complexes directly from ZnO. The resulting complexes were characterized via 1H nuclear magnetic resonance (NMR) spectroscopy and single crystal x-ray diffractometry (scXRD), which confirmed the presence of monomeric hydrated zinc acetylacetonates. Their thermal properties were evaluated via thermogravimetric analysis (TGA) to determine their thermal stability and volatility, both of which are key parameters for ALD. Furthermore, because ZnO serves as the zinc source, this approach provides insight into which acetylacetone derivatives may be most suitable for ALE of ZnO surfaces.

Session 7: Emerging Materials for biological applications

(Chair : Robert Steward)

Invited Talk: Biopolymer-van der Waals heterogeneous structures

Shuai Zhang, PNNL; Wenhao Zhou, University of Washington, Chenyang Shi, PNNL; Jiajun Chen, UW; Chunlong Chen, PNNL, Jim De Yoreo, PNNL.

Biopolymers with programmable sequences and side-chain chemistry are essential building blocks for creating hierarchical materials with diverse applications, such as microelectronics, quantum information, and biocatalysis. Recently, there has been increased interest in designing heterogeneous interfaces of sequence-defined biopolymers, like peptides, and 2D van der Waals (vdW). Inspired by nature, peptides can form various 2D supermolecular structures, like films and lamellae, with differences in order and crystallinity in response to environmental stimuli and the interfacial properties of vdW surfaces. The molecular packing and folding within these highly ordered arrays can, in turn, influence the 2D electronic confinement and charge transport across the biopolymer-vdW heterostructures. As a result, the ability to design and control biopolymer-vdW interfaces could lead to the development of new materials across multiple fields. However, a comprehensive understanding of how these biomolecules hierarchically organize on vdW surfaces is still lacking. Challenges persist in controlling assembly structures through environmental factors and exploring the energy landscape that influences different assembly phases. Additionally, the principles for achieving the desired electronic properties with programmable biopolymer assembly on vdW surfaces remain unknown. In recent years, we have concentrated on creating biopolymer-vdW heterogeneous structures with tunable hierarchies and studying their assembly dynamics using in situ atomic force microscopy, as well as understanding their specific electronic properties. In this talk, I will explain the roles of peptide-peptide and peptide-VdW interactions, along with peptide intermolecular folding and phase transitions, in regulating the assembly dynamics, order, and tailored electronic features of these heterogeneous structures. Additionally, I will showcase work on designing and synthesizing peptoids, a peptide mimetic capable of solvent-mediated (pH and cations) assembly on graphite and MoS_2, enabling controllable order, including high-crystallinity monolayer hybrid films, vesicles, lamellae, and multilayer ribbons. Our research significantly advances the understanding of designing hierarchical architectures with biomolecules at VdW-solvent interfaces, opening promising possibilities to enhance the performance of biopolymer-2D VdW hybrid materials for energy transfer, microelectronics, and quantum information applications.

Label-free optical recording of bioelectric potentials with 2D excitonic devices

Viktoryia Shautsova, University of Central Florida, Stanford University; Ashley Saunders, Stanford University; Erica Liu, Stanford University; Yang Yang, Stanford University; Edmundo Leiva, Stanford University; Nicholas Melosh, Stanford University;

Fang Liu, Stanford University; Mark Brongersma, Stanford University; Bianxiao Cui, Stanford University.

Optical imaging methods have revolutionized neuroscience by enabling systematic recordings of neuronal circuits in cultured models and in living animals. Voltage-sensitive fluorescent probes have enabled subcellular recording resolution while offering high temporal resolution. However, at high frame rate the recording duration is often limited due to photobleaching and phototoxicity of fluorescence-based voltage sensors. Label-free optical imaging approaches seek to overcome these limitations by recording neural activity without incorporating exogenous chromophores that may perturb the physiology of the cells. One such approach utilizes the sensitivity of substrate materials that change their optical properties upon neural cell firing. We previously demonstrated that two-dimensional graphene layers [1,2] and electrochromic polymer materials [3] are good candidates for such substrate materials providing high signal-to-noise ratio and high temporal and spatial resolution. However, the signal detection in these materials is based on optical reflection which requires additional optical setup design. In this work, we propose the photoluminescence-based recording of bioelectrical signals which is directly compatible with confocal fluorescence microscopes. In this poster, we will present our recent results on development of such devices that utilise 2D excitonic materials. These devices demonstrate high sensitivity of photoluminescence to local charge perturbations with $\Delta F/F0$ modulation reaching 1% for 1mV which is comparable with voltage indicators. Additionally, we will discuss the challenges of in vitro neural cultures on top of 2D materials.

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How molybdenum disulfide (MoS2) modulates actin assembly kinetics and NIH-3T3 fibroblast cell morphology and spreading

Bryan Demosthene, University of Central Florida; Tristen Gerren, University of Central Florida; Dylan Jeff, University of Central Florida; Saiful Khondaker, University of Central Florida; Ellen H. Kang, University of Central Florida

The actin cytoskeleton is active biological networks that change in response to the cell's microenvironment allowing for vital functions such as cell motility, division, and maintaining cell morphology. Molybdenum disulfide (MoS2) is a 2D transition metal dichalcogenide nanomaterial utilized in various biomedical applications due to its biocompatibility, electrochemical, and mechanical properties. The use of MoS2 in these applications increases the need to determine how these specific nanomaterials influence biological molecule structure and functions. While previous studies have shown the effects of MoS2 at the cellular level, it is not well established how MoS2 directly influences the actin cytoskeleton. In this study, we investigate the effects of MoS2 on actin cytoskeletal dynamics in the cell and determine how MoS2 modulates

actin filament assembly kinetics. Using total internal reflection fluorescence microscopy, we determined how varying concentrations of MoS2 nanoflakes influence the elongation rate of individual actin filaments. We studied changes in NIH-3T3 mouse fibroblast viability, morphology, and spreading in response to MoS2 nanomaterials. Our results showed an increase in cell spreading without a significant change in cell viability after MoS2 treatment. These results indicate that the MoS2 nanoflakes can modulate the actin cytoskeleton without inducing adverse effects on the cell depending on the concentration, leading to more safe uses of MoS2 nanomaterials in biomedical applications.

Production of MoS2 Monolayers via Peptide-Driven Liquid Phase Exfoliation

Micah Wilkerson, University of Central Florida; Dylan Jeff, University of Central Florida; Joeseph Berger, University of Central Florida; Saiful Khondaker, University of Central Florida; Lorraine Leon, University of Central Florida

Quantum materials are valued for their exceptional electronic, optical, and catalytic properties. Recent reports of bio-inspired exfoliation methods have proven successful in producing individual monolayer sheets of MoS2, enabling enhanced functionalities from an increase in surface area and interfacial interactions. Biomolecule adsorption on the surface of a quantum material fosters a new sustainable and biocompatible method, enabling tailored functionalization and self-assembly at the material surface. This study is designed to replicate the results of peptide sequence YSATFTY, which yields uniform monolayers of MoS2 and investigates the exfoliation properties of peptide sequence LEYLLEYLL. LEYLLEYLL is capable of binding to the 2d quantum material MoS2 but has unknown exfoliation properties. Both YSATFTY and LEYLLEYLL are synthesized using solid phase peptide synthesis. Liquid phase exfoliation is employed to create a peptide-MoS2 solution. The solution is sonicated, introducing mechanical agitation, assisting in the removal of the layers from the bulk material. Analysis of secondary structure, solubility, and behavior at the interface are conducted to characterize both peptides. At high concentrations, peptide aggregation affected both the secondary structure and solubility behavior confirmed by circular dichroism analysis and turbidity studies. Increasing concentration promotes intermolecular interactions, and a shift from random coil to beta sheet is observed. Nearing the critical concentration, peptide conformation transition is driven by these interactions, and self-assemble into a more ordered state. Understanding the intermolecular interactions between the peptides and MoS2 will allow the creation of advanced systems with valuable properties for applications in medicine, drug delivery, electronics, and optics.

Engineering Two-Dimensional MoS_2 Flakes to Probe Cellular Force Dynamics in Mechanobiology

Tamar Yuval Yishay, University of Central Florida; Bryan Demosthene, University of Central Florida; Dylan A. Jeff, University of Central Florida; Ellen Kang, University of

Central Florida; Saiful I. Khondaker, University of Central Florida; Robert L. Steward, University of Central Florida

Molybdenum disulfide (MoS_2) has emerged as a multifunctional quantum material in bioelectronics, biosensing, energy harvesting, and storage due to its tunable bandgap, electrical conductivity, biocompatibility, and mechano-electrical transduction. Its integration into triboelectric nanogenerators, biosensors, and hybrid energy systems highlights the importance of understanding how its physicochemical properties interact with living cells. The effects of MoS_2 on cellular forces and mechanical homeostasis remain poorly understood, limiting its application in mechanobiology. Here, we developed a systematic approach to process MoS_2 flakes into nanoscale particles for cellular mechanics studies by evaluating dispersion in Type I water and 45% ethanol and by varying the sonication method and time. MoS_2 flakes were prepared via probe or bath sonication for different durations, then lyophilized. MoS_2 prepared by 1-hour probe sonication in 45% ethanol was selected for subsequent studies due to high exfoliation rates, yielding 110–213 nm particles at controlled concentrations. HeLa cells were incubated with 25, 50, and 100 µg/mL MoS_2 at 37 °C for 24 hours to assess dose-dependent mechanical responses, as cellular mechanical dysfunction underlies diverse pathophysiological conditions, including cancer progression and tissue degeneration. By exploiting the surface area–volume ratio of MoS_2 and modulating dose, this work establishes a framework for the development and integration of two-dimensional materials in biomedical applications and biointerface design.

Poster Session Abstracts

#1 MoS_2 Interactions with HeLa Cells: Evaluating Cytotoxicity, Morphology, and Motility

Derek Freitas, University of Central Florida; Dylan Jeff, University of Central Florida; Bryan Demosthene, University of Central Florida; Tamar Yishay, University of Central Florida; Saiful Khondaker, University of Central Florida; Ellen Kang, University of Central Florida; Robert Steward, University of Central Florida

Molybdenum disulfide (MoS_2) is a transition metal dichalcogenide that has traditionally been used as a lubricant catalyst and additive in industrial and electronic application, but its potential for biomedical applications, such as drug delivery and biosensing have not yet been fully explored. MoS_2 have several advantageous properties, including semiconducting behavior, a high surface area, and photothermal capability. Although these promising properties exist with MoS_2, its effect on mammalian cell viability, morphology, and motility have yet to be established, which is important because understanding its biocompatibility is essential for evaluating its potential biomedical applications. This study aims toward evaluating the impact MoS_2 has on HeLa cells through analysis of cytotoxicity, motility, and morphology. HeLa cells were exposed to MoS_2 concentrations of 5 µg/mL, 25 µg/mL, 50 µg/mL, 100 µg/mL, and 200 µg/mL at

incubation periods of 24 and 48 hours. The average particle size of MoS_2 was 110 nm, which was measured by a particle analyzer. Cell viability was tested by using the WST-1 Assay, which measures cellular metabolic activity by monitoring mitochondrial enzyme function. Cell morphology was assessed through phalloidin staining, which labels filamentous actin to visualize cytoskeleton, and was quantified using image j. The five morphological characteristics that were assessed are area, perimeter, circumference, aspect ratio, and solidity. Migration studies were also performed to analyze migration. The results of cytotoxicity of MoS_2 on HeLa cells show no change in cell viability. Cell morphology studies show no consistent distinguishable change in morphology of the cells. The velocity studies have been conducted but have yet to be analyzed. Current results suggest MoS_2 having minimal effects on HeLa cell viability and morphology, with further analysis of cell migration continuing.

#2 Peptide-Functionalized Molybdenum Disulfide (MoS_2) Effects on Focal Adhesion Proteins in HeLa Cells

Tomas R. Martinez Grant, University of Central Florida; Dylan Jeff, College of Sciences; Angel Santos, University of Central Florida; Barbara Stewart, University of Central Florida; Nicole Verity, College of Medicine; Saiful Khondaker, College of Sciences, Nanoscience Technology Center; Lorraine Leon, College of Engineering and Computer Science; Robert Steward, College of Engineering and Computer Science, College of Medicine.

Two-dimensional nanomaterials such as molybdenum disulfide (MoS_2) have gained considerable attention in the biomedical field due to its unique properties. Its high surface-area-to-volume ratio and layered structure for accessible exfoliation are among its unique characteristics as a potential candidate for drug delivery and cell-interface engineering. Previous studies have suggested that MoS_2 may influence cellular adhesion and morphology through interactions with the actin cytoskeleton and cell-matrix adhesion proteins, such as focal adhesion kinase (FAK) and its phosphorylated state, pFAK. However, the specific effect of MoS_2 on FAK and pFAK expression and the biochemical signaling dynamics remain underexplored. The objective of this study is to determine how MoS_2 functionalized with a custom peptide designed to enhance MoS_2-to-cell surface adhesion affects the signaling dynamics of actin, FAK, and pFAK in HeLa cells. To determine how the MoS_2 and the peptide affect the signaling dynamics and cytoskeletal organization of actin, FAK, and pFAK, MoS_2 was exfoliated onto glass-bottom petri dishes and incubated with the custom peptide for one hour at room temperature to allow the peptide to bind to the MoS_2 surface. HeLa cells were then seeded onto the petri dishes mentioned above and placed in an incubator for at least 24 hours. After this time, the cells were fixed and labeled via immunocytochemistry for phosphorylated focal adhesion kinase (pFAK), total FAK, and actin filaments. The results we present here are a quantitative analysis of immunofluorescence images that display specific changes in focal adhesion and cytoskeletal distribution and morphology. This work attempts to further increase our understanding of how MoS_2 functionalized with our custom peptide influences focal adhesion dynamics and signaling pathways. These findings will integrate nanomaterial engineering and cell biology, providing

valuable information of the potential development of biocompatible platforms for therapeutic and diagnostic applications.

 # 3 The Effect of Peptide Modifications on Secondary Structure

Joseph Berger, University of Central Florida, Micah Wilkerson, University of Central Florida, Lorraine Leon, University of Central Florida

Molybdenum disulfide (MoS2) is a quantum material with potential applications as sensors or drug delivery systems. The peptide LEYLLEYLL (Leu-Glu-Tyr-Leu-Leu-Glu-Tyr-Leu-Leu) binds to MoS_2 allowing the introduction of additional functionality such as cell binding or fluorescence. The LEYLLEYLL sequence is not naturally occurring and can be synthesized using solid phase peptide synthesis (SPPS). It is unknown if small synthetic changes can create conformational shifts in the peptide that ensure stable interactions and effective binding in different biological environments. To learn more about the influence of amidated and nonamidated resin on secondary structure, two peptides were synthesized with the LEYLLEYLL sequence. One with an amide group at the C terminus (amidated), and one with a free carboxylic acid at the C-terminus (nonamidated). Circular Dichroism (CD) was used to analyze each peptide's behavior. Results from the CD showed that each peptide had a secondary structure of a random coil. This data indicates that peptide amidation did not influence peptide secondary structure. Other factors such as the concentration of peptide in solution, the addition of a fluorescent dye, and the addition of cell binding epitopes will be the focus of future experiments aimed at manipulating peptide structure and MoS_2 binding.

#4 Design of a Molybdenum Disulfide Antibody Biosensing Platform for Cancer Detection

Veeraputt DeLong, University of Central Florida; Dylan A. Jeff, University of Central Florida; Saiful I. Khondaker, University of Central Florida; Robert L. Steward, University of Central Florida

Early and accurate cancer detection remains one of the greatest challenges in modern medicine, as current biopsy-based diagnostic methods are invasive, time-consuming, and limited in their ability to provide real-time monitoring. To address these limitations, this project proposes the design of a molybdenum disulfide (MoS_2) based biosensor functionalized with half antibodies to enable direct binding and detection of cancer cells. MoS_2 offers a high surface area, strong biomolecular affinity, and tunable electrical properties, making it an excellent candidate for next-generation biosensing applications. The proposed platform employs tris(2-carboxyethyl) phosphine (TCEP) reduction to cleave full antibodies into half antibodies, exposing free thiol groups on the hinge region. These thiol groups form oriented and stable bonds with the MoS_2 surface, improving antibody orientation, antigen accessibility, and overall binding sensitivity. Characterization will be conducted using SDS-PAGE to confirm successful antibody reduction and fluorescence microscopy to visualize and quantify direct cancer cell attachment to the functionalized MoS_2 surface. The expected outcome is a biosensor with enhanced selectivity and sensitivity toward target cancer cells, providing a foundation for a minimally invasive, label-free diagnostic platform. This study aims to advance the application of two-dimensional materials in biomedical sensing and contribute toward the development of rapid, cost-effective tools for early cancer detection and monitoring.

#5 The Effects on Actin Filament Polymerization Induced by Molybdenum Disulfide (MoS_2)

Tristen Gerren, University of Central Florida; Bryan Demosthene, University of Central Florida; Dylan Jeff, University of Central Florida; Saiful Khondaker, University of Central Florida; Ellen H. Kang, University of Central Florida

Actin is a highly conserved cytoskeletal protein that polymerizes into filaments to drive key cellular behaviors, including motility, shape control, and intracellular transport.Two-dimensional molybdenum disulfide (MoS_2) nanomaterials are a metal dichalcogenide that possess distinct mechanical and surface chemistry properties, making them promising tools for interfacing with biomolecules. Previous studies have reported the cellular effects of MoS_2, but its direct impact on the actin cytoskeleton remains poorly defined. Here, we examined how MoS_2 nanoflakes affect actin cytoskeletal dynamics and filament assembly kinetics in cells. Using total internal reflection fluorescence (TIRF) microscopy, we measured the elongation rates of individual actin filaments exposed to varying concentrations of MoS_2 nanoflakes. Concurrently, NIH-3T3 mouse fibroblasts were assayed for viability, morphology, and spreading following MoS_2 treatment. Treatment produced enhanced cell spreading without a significant change in cell viability, indicating that, in a concentration-dependent manner, MoS_2 nanoflakes can modulate the actin cytoskeleton while not inducing overt cytotoxicity. These findings support the considered use of MoS_2 in biomedical applications.

#6 Influence of molecular structure on Ruthenium Atomic Layer Deposition.

Terrick McNealy-James, University of Central Florida, Xin Kang, University of Florida; Johnathon M. Johnson, University of Florida, Luis Tomar, University of Central Florida; S. Novia Berriel, University of Central Florida; Maahir Rahi, University of Central Florida; Taylor M. Currie, University of Central Florida, Titel Jurca, University of Central Florida; Lisa McElwee-White, University of Florida, Parag Banerjee, University of Central Florida

The need for alternative interconnect materials has motivated the study of Ruthenium (Ru), which exhibits excellent low bulk resistivity and surface stability. Prior investigations have utilized chemical vapor deposition (CVD) and atomic layer deposition (ALD) in augmenting film properties or performance in conjunction with Ru precursors such as: bis(cyclopentadienyl)ruthenium [$RuCp_2$], tris(2,2,6,6-tetramethyl-3,5-heptanedionato)- ruthenium [$Ru(thd)_3$] and η^4-2,3-dimethylbutadiene ruthenium tricarbonyl [$Ru(DMBD)(CO)_3$].

This study focuses on the exploration of the deposition process characteristics of Ru thin films from (η^4-diene)Ru(CO)3 complexes and film properties. Three molecules are chosen i) η^4-isoprene ruthenium tricarbonyl, ii) (η^4-1,3-butadiene) ruthenium tricarbonyl and iii) (η^4-1,3-cyclohexadiene) ruthenium tricarbonyl; with the purpose of studying the effect of changes to the ligand motif on the film growth characteristics and resulting properties in determining whether modifying the molecular structure of the Ru precursor could enable the production of films with more desirable properties. Utilizing simultaneous in situ spectroscopic ellipsometry (SE) and quadrupole mass spectrometry (QMS) during the deposition, we discern the physical growth mechanisms and chemical reactions occurring at the substrate surface. The resulting Ru grown film properties are characterized ex situ via x-ray photoelectron spectroscopy (XPS), x-ray diffraction (XRD) and four-point probe resistivity measurements.

All three candidates volatilize between 117–146 °C with film growth initiating at temperatures ≥ 180 °C. In situ SE and QMS indicate that deposition proceeds by a thermally activated spontaneous dissociation reaction with no evidence of ALD-like saturation. A pulsing sequence at a temperature of 300 °C results in a linear growth per cycle. Ex situ XPS and XRD show the formation of a nanocrystalline Ru/RuO_x mixture and 5–13 wt % C, including relatively high film resistivities measured (146–383 μΩ·cm). Ultimately, modifying the diene ligand in (η^4-diene)$Ru(CO)_3$ provides limited leverage over ALD/CVD growth behavior when H_2O is used as the co-reactant.

#7 Facet-Engineered Cu Nanocatalysts for Enhanced Nitrate Electroreduction to Ammonia

Shaurice Kildare, University of Central Florida; Zhen Meng, University of Central Florida; Xiaofeng Feng, University of Central Florida

Electrochemical nitrate reduction reaction (NO3RR) emerges as a promising strategy for the denitrification of wastewater and sustainable ammonia production. Development of such a process requires active and selective electrocatalysts for nitrate conversion to ammonia. Here we report a Cu nanoflakes electrocatalyst for nitrate reduction that was prepared with tunable morphology and facets on a Cu foam substrate. Compared to Cu nanowires, the Cu nanoflakes achieved a 5-fold increase in the activity with 81% Faradaic efficiency for NH3 production at a low overpotential of +0.15 V vs RHE. Furthermore, the intrinsic (surface-area-normalized) activity for NO3RR on Cu nanoflakes was three-times higher than that of Cu nanowires, which is attributed to the optimal ratio of exposed Cu (100) and (111) facets with synergistic effects. The Cu nanoflakes electrode was further evaluated in a single-pass flow cell for continuous nitrate electrolysis, which achieved a 97% single-pass conversion for various nitrate concentrations (1 to 50 mM) while maintaining a Faradaic efficiency of >90% for ammonia production at 0 V vs RHE. Moreover, the Cu nanoflakes showed an excellent long-term stability with 98% ammonia Faradaic efficiency and 100% single-pass conversion of nitrate, demonstrating a great promise for practical application in wastewater treatment and sustainable ammonia production.

#8 First Principle Study of Mechanical Degradation in Sulfide Solid Electrolytes: The Role of Li-Ion Concentration.

Zakariya Mohayman, Dalia Coffman, Akuhiro Kushima

All-solid-state batteries (ASSBs) utilizing sulfide solid electrolytes are considered a promising alternative to traditional lithium-ion batteries due to their high lithium-ion conductivity, modulus, and chemical compatibility with lithium metal anodes. These characteristics are anticipated to inhibit lithium penetration within the electrolyte and prevent cell short-circuiting. Nonetheless, instances of lithium penetration occurring within sulfide-based electrolytes during battery operation have been reported. One of the major reasons this happens is the mechanical degradation of solid electrolytes during battery operations. In this study, using first-principles atomistic simulations, we investigate the impact of lithium-ion (Li^+) concentration on the mechanical properties of sulfide-based solid electrolytes Li6PS5Cl (LPS). By systematically varying the concentrations of Li^+ ions, we aim to explore how different levels of ion removal/addition influence the mechanical stability and performance of the solid electrolyte. Our analysis focuses on key mechanical properties such as elastic modulus, tensile strength, and fracture toughness. By simulating and analyzing the deformation of computational cells across various lithium concentrations, this study identifies a critical relationship between lithium concentration and the deterioration of mechanical properties. This deterioration is implicated as a potential cause of mechanical failure in ASSBs. We also perform a comparative study with the effects of electrochemical reactions of LPSCl by altering Li atomic concentration to provide a comprehensive understanding of the structural and mechanical implications at the solid electrolyte grain boundaries and electrode interface. The results showed a significantly more reduction in the mechanical strength when there is a decrease in the Li+ concentration. This indicates that LPSCl may have internal weak spots that can lead to fracture and promote lithium metal penetration. The findings from this research contribute to understanding the root cause of ASSB failure and the optimization and design of sulfide-based solid electrolytes for advanced battery technologies, potentially leading to improved performance and longevity of next-generation energy storage systems.

#9 Comparison of Experimental Analysis and Theoretical Calculation of the Lattice Dynamics, Phonon and Vibrational Spectra Dynamics of Titanium Nitride and Oxynitride

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State University; J. David Schall, Department of Mechanical Engineering, North Carolina A&T State University; and Dhananjay Kumar, Department of Mechanical Engineering, North Carolina A&T State University

Titanium nitride (TiN) and its isostructural oxide derivative, Titanium oxynitride (TiNO) has gained interest in industry as a cost-effective alternative material to noble metals and refractory metals with wide range of applications especially in the optoelectronics and plasmonic. However, there still remain some gaps and disagreement in the literature on specific optical and photoelectrochemical properties of TiN and TiNO, due to difficulty and the varying approach in quantifying defects, vacancies, oxidation state and direct impact of impurities in experimental results.

In this study, a novel on-lattice sampling approach and Molecular Dynamics (MD) is used to generate TiN and TiNO structures that compare well with single crystal synthesized thin films (grown with the pulsed laser deposition technique on sapphire-Al2O3). Structural properties of these thin films were investigated using X-ray Diffraction and Reflection (XRD, XRR), X-ray Photoelectron Spectroscopy (XPS), Rutherford backscattering spectrometry (RBS), Raman Spectroscopy and Fourier Transform Infrared Spectroscopy (FTIR); and these results are compared with the calculated phonon dispersion and infrared absorption bands to provide understanding the effects that various property variations such as oxygen-dependent semiconductivity, defect/vacancy formation, symmetry of phonon bands, etc. on the optical and plasmonic properties of TiN and TiNO material system.

To corroborate our experimental observations, the phonon dispersions and Raman active modes are calculated by using the virtual crystal approximation for rutile TiO2 and rocksalt TiNO, which shows that the incorporation of nitrogen atoms does not significantly alter the phonon dispersions of rutile TiO2. However, it results in the emergence of new phonon modes at approximately 7.128 THz (237.65 cm-1) at the Gamma point, which corresponds to the experimentally observed Multi-Photon Phase-MPP (240 cm-1-R). From the experimental and theoretical studies, a multilayer optical model has been proposed for the TiN/TiNO epitaxial thin films for obtaining individual complex dielectric functions from which many other optical parameters can be calculated.

This work was supported by a DOE EFRC on the Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS) via grant # DE-SC0023415. Part of the work has used resources established by the Center for Collaborative Research and Education in Advanced Materials (CREAM) via NSF PREM grant # DMR-425119 PREM. ML is jointly supported by the CEDARS and CREAM projects.

#10 In Situ Mass Spectrometry During Powder Atomic Layer Deposition for Surface Reaction Analysis on ZnO Nanoparticles

Ayelen Mora, University of Central Florida; Eric Bissell, University of Central Florida; Parag Banerjee, University of Central Florida.

Quantum nanoparticles are unique because of the electrical and optical properties they exhibit as a result of quantum confinement. However, decreasing particle size in turn increases surface area. Without surface passivation, the high amount of surface defects and dangling bond defects that result from this increased surface area accelerate degradation and reduce device performance. Atomic layer deposition (ALD) offers a means to apply this surface passivation. With its sequential, self-limiting surface reactions, ALD can deposit thin conformal coatings that passivate the defect sites leading to improved performance. However, the extension of ALD to high surface area nanoparticles systems presents unique challenges, including precursor diffusion limitations, particle agglomeration, and extremely high surface areas (reaching ~10s of m^2/g). These factors complicate the process, making it essential to monitor reaction progress and identify saturation ("end-pointing") within the powder bed. In this work, we employ quadrupole mass spectrometry (QMS) as an in situ diagnostic tool to study Al_2O_3 ALD on ZnO nanoparticle powder beds. Using trimethylaluminum (TMA) and ozone (O_3) as precursors at a deposition temperature of 120 °C, we track methane (CH_4) evolution—a key reaction byproduct—to gain insights into surface reaction kinetics and saturation behavior. Furthermore, we develop multivariate analysis tools to interpret ALD reaction dynamics in powder bed reactors with the hope of enabling better process control.

 # 11 Effect of lattice strain on adsorption properties of metal nanoclusters on boron phosphide substrate

Ruthlyn Mangroo, University of Central Florida; Zakariya Mohayman, University of Central Florida; Akihiro Kushima, University of Central Florida;

Development of high-performance catalyst is crucial for advancing sustainable energy technologies and chemical transformations. Recently, nano-structured materials and novel metal clusters have been introduced for enhancing catalytic efficiency, selectivity, and stability. Here, boron phosphide (BP) films offer a unique platform to grow nano clusters (or single atom) due to their exceptional thermal stability, tunable electronic properties, and strong metal adsorption capabilities. BP films decorated with metal nano clusters has potential applications in various electrocatalytic reactions such as hydrogen evolution, CO2 reduction, alcohol oxidation, and selective hydrogenation. The adsorbed metal clusters possess different structure than their bulk counter parts due to the size-scales altering their physical properties. The structures of BP layer can also be modified by creating heterostructures combined with different substrate and controlling the in-plane lattice strains, which leads to further tunability of the metal cluster catalysts. In this work, first-principles atomistic simulations are performed to study the adsorption structure and energy of different novel metals on BP surface under different in-plane strains. The metal clusters showed excellent binding on BP film with large deviations from the bulk structures. The information obtained in this work contributes to developing novel composite catalysts with high stability and tunability, which allows optimization of the catalytic properties for various applications.

#12 Atomic Layer Deposition of Er-doped CeO_2 for Quantum Information Processing

Terrick Mcnealy-James, University of Central Florida; Emily Miura-Stempe, University of Washington; Brandi M. Cossairt, University of Washington; Parag Banerjee, University of Central Florida.

Erbium-doped cerium oxide (Er:CeO_2) has emerged as a compelling solid-state material for spin-based quantum information processing, due to CeO_2 crystalline morphology, wide band gap(3.19 eV) and low concentration of nuclear spins. Recently, Er:CeO_2 nanoparticles have demonstrated long electron spin coherence times in the microsecond range. However, their discrete morphology and particulate form pose challenges for large scale integration into solid-state device architectures.

In this work, we address these challenge by demonstrating the synthesis of Er:CeO_2 thin films using atomic layer deposition (ALD), a gas phase, wafer scale technique capable of sub-monolayer dopant control and conformal coating. ALD of CeO_2 is based on our Group's previous work using the commercial precursor Ce(iPrCp)2(N-iPr-amd) (Celine) with O_2 plasma. The Er_2O_3 process utilizes tris(methylcyclopentadienyl)erbium ((CpMe)3Er) as the Er precursor and O_2 plasma as the oxidant. 5 Films are deposited through alternating pulses of Celine and O_2 plasma with intermittent pulses of (CpMe)3Er and O_2 plasma to incorporate Er_2O_3 into the CeO_2 matrix. By exploiting the steric hindrance and controlled under-dosing during the Er pulses, lateral spacing between ions within the CeO_2 matrix is maintained, while vertical separation is maintained by the addition of CeO_2 layers between successive Er_2O_3 layers.

Growth is monitored in situ using simultaneous spectroscopic ellipsometry (SE) and quadruple mass spectrometry (QMS). SE provides real-time information on film thickness, refractive index and optical properties, enabling the identification of growth regimes and surface reactions with sub-monolayer sensitivity. Concurrently, QMS tracks the evolution of gas-phase species and reaction by-products, providing insight into precursor decomposition pathways and surface reactions.

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#13 Unconventional Semiconductors as Catalytic Supports: Synthetic Strategies and Noble Metal Integration

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Semiconductors, while traditionally associated with electronic and optoelectronic applications, are increasingly recognized for their potential as supports in heterogeneous catalysis. Conventional noble metal catalysts exhibit excellent activity and selectivity; however, their large-scale deployment is constrained by high costs, limited availability, and volatility in global supply chains. One promising strategy to address these challenges is the deposition of catalytic metals onto large scale nano-to-micro particulate supports. Under this broad scope, semiconducting supports can simultaneously reduce noble metal loading and potentially exploit the unique electronic properties of semiconductors to enhance catalytic performance.

In this study, we investigate boron phosphide (BP), indium phosphide (InP), and bismuth telluride (Bi2Te3) as unconventional semiconductor-type supports whose catalytic potential remain largely unexplored. Each material presents distinct opportunities and challenges. BP, despite its favorable electronic structure, has received limited attention due to the synthetic difficulties arising from boron’s chemical inertness. InP has been extensively studied in photonics, particularly in the form of quantum dots, but its nanoscale manifestations are unsuitable as catalyst supports, necessitating scalable bulk synthesis. Bi2Te3, widely investigated for thermoelectric and photovoltaic applications, is also a prototypical topological insulator with protected surface states that may facilitate charge transfer processes. Despite these unique attributes, it has not yet been systematically evaluated as a catalytic support, even though its tunable band structure and strong light–matter interactions suggest significant promise.

Our initial objective is to establish green, scalable, and reproducible synthetic routes for bulk BP, InP, and Bi2Te3. To this end, we are adapting and refining protocols from literature [1, 2, 3]. Thus far, we have achieved phase-pure BP via a mechanochemical route and crystalline Bi2Te3 through solvothermal synthesis. Current efforts are directed toward optimizing sonochemical methods for InP to improve yield and scale of the reaction. By integrating semiconductor specific properties with noble metal catalysis, this work aims to establish a new class of cost effective, efficient, and robust catalytic systems. Ultimately, our findings will provide fundamental insights into the role of semiconducting supports in heterogeneous catalysis and open pathways toward sustainable catalyst design.

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#14 Electronic Band Structure of a Nodal Line Semimetal Candidate ErSbTe

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The lanthanide-based antimony tellurides (LnSbTe, Ln = lanthanides) exhibit rich physics driven by the interplay of crystalline symmetry, magnetic ordering, 4f correlations, and spin–orbit coupling (SOC). We investigate the nodal-line semimetal candidate ErSbTe through combined transport, thermodynamic, and angle-resolved photoemission spectroscopy (ARPES) studies, supported by first-principles calculations with and without SOC. ErSbTe hosts a diamond-shaped Fermi surface with band crossings along Γ–X protected by nonsymmorphic symmetry, forming part of a nodal line along X–R, while a secondary crossing becomes gapped along Γ–M. Magnetic susceptibility, resistivity, and heat-capacity measurements reveal a paramagnetic-to-antiferromagnetic transition near 1.94 K and an additional anomaly at 1.75 K, without

the hump-like resistivity feature seen in related compounds. These findings identify ErSbTe as a distinct member of the LnSbTe family, where symmetry, SOC, and magnetism collectively define its emergent properties.

#15 Electronic structure of a layered altermagnetic compound CoNb4Se8

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Altermagnets (AMs) have recently emerged as a promising class of magnetic materials characterized by unique spin-splitting even in the absence of both net magnetic moments and spin-orbit coupling. Despite numerous theoretical predictions, experimental evidence of such spin-splitting in real materials remains limited. In this study, we use angle-resolved photoemission spectroscopy (ARPES) combined with density functional theory (DFT) calculations to investigate the electronic band structure of the altermagnet candidate CoNb4Se8. This material features an ordered sublattice of intercalated Co atoms within NbSe2 layers. Magnetization and electrical resistivity measurements reveal the onset of antiferromagnetism below 168 K. Temperature-dependent ARPES data, supported by DFT calculations, uncover spin-split bands along the M–Γ–M high-symmetry direction. The observation of spin-splitting in this high-temperature altermagnet opens new avenues for exploring its electronic properties and potential applications in spintronic technologies.

#16 A Python-Based Approach for Real-Time Data Analysis of Tr-ARPES

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Kagome lattice systems, composed of corner-sharing triangles arranged in a star-of-David pattern, offer a compelling platform for exploring the interplay between lattice, geometry and correlated electronic phenomena. These materials are known to host exotic features such as flat bands, Dirac crossings, and van Hove singularities, making them an ideal candidate for investigating emergent quantum behavior. In this study, we present a preliminary investigation of ultrafast phenomena on Kagome materials - TbMn6Sn6 and YMn6Sn4Ge2, using time and angle resolved photoemission spectroscopy (Tr-ARPES). We visualize ultrafast dynamics using Igor Pro, the widely adopted tool for ARPES data analysis, and introduce an open-source Python-based analysis framework using the PyARPES library. We describe the steps taken to convert raw ARPES data into a format accessible by Python and outline future directions for incorporating advanced

visualizations, such as identifying quasiparticle interaction and associated timescale, Fermi level shift, and electronic temperature (Te). Finally, we discuss our long–term goal of leveraging Python for incorporating artificial intelligence into ARPES and Tr-ARPES studies for real-time data analysis and predicting various competing orders and quantum phenomena.

#17 Preliminary Transport Measurements for Rare-Earth-Based Topological Nodal-line Semimetal Candidate

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Magnetic topological semimetals are notable for possessing remarkable transverse transport properties, large non-saturating magnetoresistance, and anomalous spin textures. The LnSbTe family of materials, where Ln is in the Lanthanide series, are well-known magnetic topological nodal line semimetals crystallizing in the tetragonal ZrSiS-type structure. Here we study a new related compound featuring a slight monoclinic distortion, the effect of which is expected to modify the pertinent symmetries involved in the topological characteristics of the material.

#18 Altermagnetic Spin-Splitting in an Intercalated Transition Metal Dichalcogenide

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Altermagnetism represents a newly recognized class of magnetic order that combines the compensated spin structure of antiferromagnets with the spin-polarized electronic states characteristic of ferromagnets. Layered materials hosting such order provide an appealing platform for exploring symmetry-governed spin phenomena and integrating magnetic functionality into low-dimensional systems. In this work, we identify and investigate an intercalated transition-metal dichalcogenide as a promising layered altermagnet. Through a combination of experimental and first-principles approaches, we probe its electronic structure and temperature evolution, revealing characteristics consistent with the emergence of altermagnetic behavior. These results highlight the potential of intercalated transition-metal dichalcogenides as a versatile materials platform for realizing and controlling altermagnetism in low-dimensional systems.

#19 Epitaxial Growth and Structural Characterization of Bi_2Te_3 Thin Films on GaAs(100) by Molecular Beam Epitaxy

Nia Suitt, Himanshu Sheokand, Madhab Neupane, University of Central Florida

Bismuth telluride (Bi_2Te_3), a prototypical topological insulator has attracted significant attention due to its layered crystal structure and tunable electronic properties. However, the growth of high-quality Bi_2Te_3 thin films remains challenging because of the narrow stoichiometric window and strong dependence on substrate orientation and growth kinetics. In this work, we report the epitaxial growth of Bi_2Te_3 thin films by molecular beam epitaxy (MBE) on GaAs(100) substrates under ultra-high-vacuum conditions. A Te-rich flux ratio was maintained to suppress Te desorption and ensure stoichiometric film formation. The evolution of in situ reflection high-energy electron diffraction (RHEED) patterns revealed a transition from streaky to well-defined (1×1) reconstructions, confirming two-dimensional layer-by-layer growth. X-ray diffraction (XRD) measurements were performed to confirm the crystallinity and c-axis orientation of the grown films, while energy-dispersive X-ray spectroscopy (EDS) verified the expected Bi_2Te_3 stoichiometry through both atomic and weight composition analysis. These results highlight the importance of flux optimization and substrate orientation in achieving high-quality Bi_2Te_3 epitaxy, paving the way for device-scale studies of topological and thermoelectric phenomena.

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#20 Electronic Band Topology in the Orthorhombically Distorted Nodal Line Semimetal Candidate CeAsS.

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Rare-earth–based materials derived from the ZrSiS family have emerged as ideal platforms to explore the interplay between magnetism, 4f-electron correlations, topological band structures and crystalline symmetry. Extending this landscape, we investigated the closely related compound CeAsS, which crystallizes in an orthorhombic Pnma structure through a combination of angle-resolved photoemission spectroscopy

(ARPES), density functional theory (DFT) calculations, and comprehensive thermodynamic and transport measurements. Magnetic susceptibility, magnetization, and specific heat measurements reveal a long-range antiferromagnetic transition at TN = 9.5 K, which shifts to lower temperature under applied field, and a field-induced phase emerging above 6 T. Electrical resistivity confirms metallic behavior, while magnetotransport measurements uncover a large, non-saturating magnetoresistance exceeding 600% at 1 K and 13 T, accompanied by Shubnikov–de Haas oscillations indicative of high carrier mobility and compensated semimetallicity. ARPES spectra collected in the paramagnetic phase display a diamond-shaped Fermi surface with distinct corner pockets and linearly dispersive surface bands forming gapless Dirac-like crossings around 150 meV below fermi level. These findings identify CeAsS as a correlated semimetal where antiferromagnetism, 4f-electron interactions, and Dirac-like dispersions coexist, providing a promising platform to study the coupling between magnetic order and topological electronic states in lanthanide pnictide-chalcogenides.

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#21 Epitaxial growth of altermagnetic α-MnTe on GaAs(111)B substrate via molecular beam epitaxy.

Himanshu Sheokand, University of Central Florida; Madhab Neupane, University of Central Florida

The altermagnetic materials has emerged as a model system for studying spin-split electronic structures, yet controlled epitaxial growth on technologically relevant substrates remains challenging. Among the known candidates, MnTe stands out as a prominent altermagnetic material owing to its layered structure and high Néel temperature. Here, we report the molecular beam epitaxy (MBE) growth of high-quality α-MnTe thin films on GaAs(111)B substrates and provide a comprehensive analysis of the growth evolution and structural properties. Real-time reflection high-energy electron diffraction (RHEED) reveals a transition from three-dimensional island nucleation to streaky two-dimensional patterns, indicating the development of smooth, epitaxial layers despite the large lattice mismatch. Raman spectroscopy confirms the formation of the hexagonal NiAs-type phase through the observation of the characteristic phonon modes at 121 cm^{-1} and 140 cm^{-1}. X-ray diffraction measurements verify single-phase (0001) orientation, while scanning electron microscopy, energy-dispersive X-ray spectroscopy, and atomic force microscopy demonstrate uniform morphology, near-stoichiometric Mn:Te composition, and nanometer-scale surface roughness. These results establish a reliable growth protocol for α-MnTe on GaAs(111)B and provide a foundational platform for exploring strain-engineered altermagnetism and spin-dependent phenomena in epitaxial MnTe heterostructures. Acknowledgement: M. N. is supported by the US

Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award DE-SC0024304.

#22 Quantum batteries: Thermodynamic foundations and design principles

Kashvi Modi, University of Central Florida; Dr. Tom Hopper, University of Central Florida

Quantum batteries (QBs) are devices that store and release energy using quantum mechanical effects instead of chemical reactions like classical batteries. Because these batteries depend on quantum mechanical effects, they can in principle charge faster with less loss of energy.1 However, the researchers face major challenges with maintaining coherence over long periods and scalability. This poster explores concepts of quantum thermodynamics and quantum chemistry that would be useful to describe energy storage at the quantum level and understand efficiency limits and discharge stability after conducting a literature review. Special attention is given to ultrafast spectroscopy and how that can potentially be used to overcome current gaps in research. The long-term goal is to develop quantum batteries that combine fast charging, low dissipation, and stable energy retention.

#23 Lattice dynamics of layered kagome lattice material Nb3Br8 investigated via Raman spectroscopy and DFT

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Niobium bromide (Nb3Br8) is a quantum material that crystallizes in a layered breathing kagome lattice with topologically flat bands, serving as a potential platform for correlated electronic states. Nb3Br8 also undergoes a structural phase transition when heated above 387 K that changes the stacking order of the lattice and induces a magnetic phase transition. Despite being a promising quantum material for the study of exotic electronic and magnetic states, an understanding of the lattice dynamics of Nb3Br8 remains elusive. In this study, exfoliated bulk and few layer Nb3Br8 flakes are investigated via linearly polarized Raman spectroscopy and density-functional theory (DFT) to study the crystal’s phonon modes and their symmetrical representations. 18 modes are resolved in exfoliated bulk, 10 are Eg modes and 8 are A1g modes, in close agreement with DFT analysis. Linearly polarized Raman spectroscopy performed above 387 K showed no changes in the Raman selection rules of the phonon modes, suggesting their insensitivity to the structural phase transition. Finally, layer-dependent Raman studies reveal that the intensity of bands in the Raman spectra decrease and experience a slight shift in frequency in thin layers, however the Raman selection rules remain consistent with bulk. This study serves to establish a foundation for future studies of Nb3Br8 and its characteristic Raman-active phonon modes across different structural phases and thicknesses down to bilayer.

#24 Substrate Effects on the CVD-Growth and Transfer of MoS2

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Molybdenum disulfide (MoS_2) is a two-dimensional quantum material that possesses unique electronic properties, making it a promising candidate for next-generation semiconductor and biological applications. Chemical vapor deposition (CVD) is a widely used method of synthesizing thin layer MoS_2, offering superior scalability and control over mechanical exfoliation. For different applications, MoS_2 needs to be grown on different substrates, and often requires post-growth transfer onto a new substrate. For example, studies of MoS_2-cell interaction require MoS_2 grown on glass or sapphire substrate. In some applications, flakes may need to be transferred onto unconventional substrates, such as photonic crystals or waveguides, where direct growth is not possible. Here we discuss our growth and transfer techniques of MoS_2 on Si/SiO_2 and glass substrates. We grow on both substrates and utilize a dry transfer method to transfer the flakes onto an arbitrary substrate. We will characterize the surface topography of both as grown and transferred flakes via Atomic Force Microscopy to better understand the effects of growing nanomaterials on different substrates.

#25 Temperature Dependent Mechanical Exfoliation of Thin layer 2D Quantum Material PdPS3

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Two-dimensional (2D) layered materials have attracted enormous interest owing to their atomic-thin structure and emergent properties that differ from their bulk analogues. $PdPS_3$, a member of the metal phosphorus trichalcogenide (MPX_3, X = S, Se) family, is of particular interest among these 2D materials because its monolayer form of is predicted to host multiple Dirac cones and exhibit topological magnetism. However, exfoliation of $PdPS_3$ and its characterization remains largely unexplored. While simple mechanical exfoliation can produce high-quality flakes, in general it gives low yields; Therefore, study of high yield exfoliation of PdPS3 is of particular interest for its potential applications in low-dimensional magnetic & spintronic devices. Here, we investigate the mechanical exfoliation of $PdPS_3$ with a focus on how substrate annealing temperature and substrate preparation affect the transfer yield and flake thickness. Building upon methods reported

for other van der Waals materials, we exfoliated bulk $PdPS_3$ crystals using adhesive tape onto Si/SiO_2 substrates subjected to controlled annealing at different temperatures while maintaining tape contact during the process. The resulting samples were characterized via optical microscopy and atomic force microscopy (AFM), to determine flake coverage and thickness distribution. By systematically varying annealing conditions, this study seeks to establish optimal parameters for producing thin $PdPS_3$ flakes and to provide insight into the adhesion and release mechanisms specific to this material. The outcomes will address a current gap in the literature concerning mechanical exfoliation of $PdPS_3$, offering a foundation for future work on its electronic and magnetic properties and enabling reproducible preparation of high-quality 2D $PdPS_3$ layers for device integration.

#26 Nanoscale Mapping of Electronic Properties of the 2D Quantum Material PdPS3 via KPFM and C-AFM

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PdPS3 is member of the transition metal phosphorus trichalcogenide (MPX3, X = S, Se) family of van der Waals materials, a broad group of materials of particular interest owing to their chemical stability and layered structure, making them attractive candidates for the investigation of nanoscale physical phenomena in quantum materials. Despite the steadily growing interest in this group of materials, the electronic properties of PdPS3, such as surface potential and local conductivity and their thickness dependence, remains unknown. This study examines the nanoscale electronic properties of mechanically exfoliated PdPS3 flakes on gold substrates through Kelvin probe force microscopy (KPFM) and conductive atomic force microscopy (C-AFM). KPFM is performed on PdPS3 flakes of different thicknesses to determine the layer-dependent contact potential difference to clarify the local differences of the electronic work function. C-AFM is utilized to generate bias-dependent maps of current on the nanoscale across different layers. The combined analysis of the data from the KPFM and C-AFM measurements helps identify correlations among surface potential, thickness, and localized current features that can be related to the transport behavior of PdPS3. Our findings not only help unravel the physics of work function variations and current transport in PdPS3, which has been less explored than its MPX3 counter parts, but will also help fill the existing gap in understanding the nanoscale properties of this family of layered quantum materials.

#27 Petahertz Lightwave Control of Quantum Interference in Graphene and Flat-Band Materials

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Time-resolved spectroscopies have revolutionized our ability to probe ultrafast processes in solids, revealing how electronic populations evolve following optical excitation. Yet, these techniques often remain blind to the phase of the electronic wavefunction, which encodes the quantum geometry, which governs charge transport, interference, and control at the sub-cycle level. To access this phase information, interferometric tools operating directly within solids and on timescales shorter than the typical electronic dephasing time of only tens of femtoseconds are required. In the prototypical model system graphene, it has been demonstrated that few-cycle light fields can coherently drive and control coupled intra- and interband dynamics, giving rise to Landau–Zener–Stückelberg–Majorana (LZSM) interferometry. Here, tunneling between valence and conduction bands acts as a light-field-controlled beam splitter for electrons. The resulting quantum trajectories interfere within the crystal, forming a solid-state analog of a Mach–Zehnder interferometer. The accumulated phase then determines the direction of the light-field-induced current. While previous experiments have employed few-cycle 800 nm pulses, we now extend this concept to single-cycle mid-infrared excitation, which enhances control and precision in reading out the interferometric phase. Beyond monolayer graphene, our focus shifts toward bilayer, flat-band systems and quantum materials beyond graphene. Furthermore, we apply out-of-plane DC fields to tune the band geometry and Berry curvature, properties that can be directly probed via LZSM interferometry. Moreover, by introducing a second, phase-locked light field as a Floquet drive, we aim to dynamically engineer transient band structures and probe their evolution interferometrically. Together, these developments establish a framework for phase-resolved quantum control in solids, enabling new ways to map quantum geometry, coherence, and topology at the petahertz frontier.

#28 Unified Symmetry Framework for Excitons in two-dimensional Quantum Materials: Monolayer and Bilayer Transition-Metal Dichalcogenides and Altermagnets

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Excitons, bound electron-holes states, often dominate the optical response of two-dimensional (2D) quantum materials and reflect their inherent properties, including spin-orbit coupling, magnetic ordering, or band topology.A unified symmetry framework for excitons provides a transparent model of exciton beyond the hydrogen picture. Such a framework predicts resonant mixing of 1s and 2p excitons when the exciton Hamiltonian commutes with a total angular momentum made possible by broken mirror symmetry in monolayer TMD or inter-layer hopping in 3R-stacked bilayer TMD[1]. In 2D Altermagnets, the symmetry of excitons is described by spin-space-group (SSG) representation theory. These excitons yield distinct polarization-dependent optical selection rules and serve as

optical fingerprints for detecting altermagnetism. Our framework also unified the description of excitons across different 2D platforms.

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#29 Enhancing the structural and plasmonic stabilities of TiO2-supported Au nanobipyramids by metal shell deposition

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Anisotropic plasmonic metal nanoparticles (NPs) show significant promise as light-sensitizing components in the design of advanced optical materials. Their plasmon resonances can be tuned across the visible and near-IR regions simply by adjusting their aspect ratio, allowing them to harvest solar energy well below the bandgaps of conventional semiconductors. By incorporating them into the structure of UV-active semiconductors, composite materials can be prepared that are capable of absorbing the bulk of the solar spectrum. However, the steps involved in material processing and the environmental conditions during real-world application frequently include elevated temperatures. Metal NPs are known to significantly restructure and change shape under thermal conditions, and for anisotropic plasmonic metal NPs this leads to a shift of their plasmon resonances, limiting their practical utility. Therefore, it is necessary to develop strategies to improve their thermal shape stability. Here, we demonstrate that the deposition of thin shells of different metals (Ag, Pd, Pt) can alter and drastically increase the thermal stability of anisotropic Au nanobipyramids (NBPs), an emergent class of Au nanocrystals with an abundance of high-index surface facets that make them highly prone to thermally induced shape change. Using a combination of solid-state UV-vis spectroscopy, transmission electron microscopy (TEM), and energy-dispersive X-ray (EDX) spectroscopy, we investigate the thermal stability of these Au@M NBPs immobilized on a TiO2 support, a popular semiconducting metal oxide frequently employed as a support material for metal NPs. While for pure Au NBPs and Au@Ag NBPs, their tips are observed to progressively blunt and their plasmon resonances begin to blue-shift when annealed at 100℃, the shapes and plasmon resonances of Au@Pd and Au@Pt NBPs are well-maintained up to 200℃ and 250℃, respectively. Notably, we also find that the thermal stability of Au@Pd and Au@Pt NBPs is unaffected by annealing time up to 4 hrs, suggesting that this method can be used to protect metal NPs in a diverse range of operating conditions. We further use EDX spectroscopy to map the alloying processes of these core@shell NBPs. The onset temperature of alloying for the different Au@M NBPs appears to increase as the lattice mismatch between core and shell metals increases.

#30 Spin-photon Defect Centers in Silicon for Scalable Quantum Technologies

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Solid-state material platforms have been instrumental in realizing spin-based qubits with long optical and spin coherence, offering a pathway toward scalable quantum technologies, including quantum processors, quantum memories, and quantum communication networks. Among these, atomic defect-based color centers such as nitrogen vacancy (NV) and silicon vacancy (SiV) center in diamond, divacancies in SiC, quantum dots in III-V semiconductors, and defects in two-dimensional materials such as hexagonal boron nitride (hBN), have demonstrated remarkable progress in spin-photon interface, single photon generation and quantum sensing. However, each of these system faces intrinsic challenges that limit scalability. Diamond and SiC centers emit outside the telecom band and require complex heterogeneous integration, while quantum dots suffer from spectral inhomogeneity and device-to-device variation. To date, no single material platform has simultaneously met the requirements for quantum processing, quantum storage, and quantum networking within a fully CMOS- compatible framework.

Recent breakthroughs in silicon-based color centers have opened a new frontier by combining telecom band emission, long spin coherence, and native integration with silicon photonics. In particular, carbon-related defects in isotopically purified silicon such as G- and T- centers have shown promising characteristics as spin-photon qubits. The T-center, for example, has enabled long-lived spin-photon entanglement and demonstration of a three-qubit register, firmly establishing silicon as a credible host for scalable quantum technologies. Building on this progress, we recently demonstrated the femtosecond-laser-assisted generation of a novel isolated Ci center in silicon, which emits at ~ 1452 nm, within a low-loss telecom band, and exhibits a spin-triplet ground state suitable for spin-photon interface.

In this work, we present the monolithic integration of Ci center with a silicon nanophotonic cavity to enhance quantum light emission efficiency and photon indistinguishability through strong light-matter interaction. We design, simulate, and fabricate nanobeam cavities with high-quality factors exceeding 10^5 and mode volume below 0.6 (λ/n)3, enabling Purcell enhanced emission and life-time reduction. The deterministic “write/ erase” placements of Ci center at the antinodes of the cavity is achieved using femtosecond-laser pulses with in-situ feedback ensuring sub-micron precision and reproducibility. The integrated devices are characterized through on-chip quantum measurements, including Hong-Ou-Mandel (HOM) experiments using off-chip superconducting nanowire detector, demonstrating photon indistinguishability.

This work establishes a fully CMOS-compatible silicon quantum photonic platform that unites nanophotonic design, simulation, fabrication, deterministic emitter creation, high-coherence spin-control, and integrated detection, representing a critical step toward large-scale, telecom band quantum processors, quantum memories and quantum networks.

#31 Petahertz Electronics: Tracking Coherent Electron and Exciton Dynamics in Quantum Materials

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Understanding and controlling coherent electron and quasiparticle dynamics in solids lies at the heart of modern condensed matter physics and ultrafast photonics. While photon-based spectroscopies such as time-resolved photoluminescence and transient absorption have revolutionized our understanding of light–matter interaction, they are intrinsically limited to probing population dynamics rather than the underlying coherent motion of charges and excitons. Capturing these sub-cycle dynamics in quantum materials, in which electronic coherence unfolds over the light oscillation period, i.e., at 100s THz frequencies, requires a new experimental tool.

In our group, we develop and apply such tools, broadly referred to as petahertz electronics, to directly track the coherent polarization and field-driven electron motion in quantum materials. By combining ultrabroadband single-to-few-cycle light pulses with field-resolved detection, we can measure the transient electric field emitted by a material with sub-femtosecond precision. This enables us to access the instantaneous polarization response of solids and excitons, opening a new window into the ultrafast buildup of coherence and collective quantum phenomena.

Building on previous results obtained in the antiferromagnetic semiconductor CrSBr, a model excitonic material exhibiting strong spin–exciton coupling and long-lived excitonic coherence, we are now extending these approaches to a broader class of quantum materials. Thereby, the CrSBr studies serve as an important benchmark, demonstrating that petahertz field-resolved spectroscopy can capture the emergence of a phase-synchronized exciton ensemble, in which individual excitons lock their optical phases through coherent coupling. We will further discuss the possibility of super-radiance.

In the second part of the talk, I will discuss how coherent many-body phenomena may lead to light-induced quantum phase transitions, in which intense optical fields dynamically modify crystallographic and electronic symmetries. Finally, I will outline how petahertz electronics can evolve into a universal platform for probing and controlling correlated quantum materials.