PCSI

Room Ballroom South - Session PCSI-SuA

Exotic Forms of Magnetism

Moderator: Scott Crooker, Los Alamos National Laboratory

3:30pm **PCSI-SuA-1 Magnon-Exciton and Magnon-Photon Couplings in CrSBr*, Eunice Bae,*** Cornell University **INVITED**

Magnon-based hybrid quantum systems are promising candidates for quantum interconnects and quantum sensors, and they offer a rich platform for exploring nonlinear magnonics and cavity–photon interactions. Two-dimensional (2D) van der Waals magnets provide a compact, atomically flat geometry that can be easily integrated into existing quantum circuits, such as superconducting resonators and qubits. Among various 2D magnets, the magnetic semiconductor CrSBr is particularly unique due to its strong spin–exciton [1, 2], spin–lattice [3], and magnon–exciton [4] interactions. In this presentation, I will first discuss magnon-exciton coupling despite their energetical mismatch by orders of magnitude. I will then discuss our recent work demonstrating coherent coupling between antiferromagnetic magnons in CrSBr and microwave photons in a niobium-based-on-chip resonator [5]. This work demonstrates the first step toward integrating layered van der Waals 2D magnets into superconducting microwave circuits, with full access for both microwave and optical probing. Finally, I will discuss how these properties of magnetic semiconductors can be harnessed for spintronic devices and quantum information science.

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[5]Tang, J., Singh, A., Brennan, N., Chica, D., Li, Y., Roy, X., Rana, F., Bae, Y.J., Coherent Magnon-Photon Coupling in the Magnetic Semiconductor, 2025, Nano Lett., 25, (2025),10912-10918.

4:10pm **PCSI-SuA-9 Developing Tkinter-Based Application for Processing Electrical Transport Data Measured in Pulsed Magnetic Fields*, Gabriel Ruiz,*** Los Alamos National Laboratory

Pulsed magnetic fields provide access to extreme field regimes that are essential for probing quantum phenomena and characterizing complex material behaviors. However, their rapid field ramping introduces substantial measurement challenges, particularly the emergence of large Faraday-induced voltages in electrical transport setups. These unwanted voltages, arising from thetime derivative of themagneticflux, can exceed the intrinsicsample signal by ordersof magnitude and result in misleading asymmetries between the up-sweep and down-sweep of the magnetic field. This artifact not only distorts critical features such as quantum oscillations and resistive transitions but also complicates post-experimental analysis. To address this issue, we developed a Python-based software tool equipped with a graphical user interface(GUI) using the Tkinter library. The program enables users to automatically correct for the Faraday-induced voltage component by leveraging the inherentant isymmetry of the induced sign al between rising and falling field sweeps. It applies a least-squares fitting algorithm to extract normalization coefficients ($A_x$and A_Y) that best describe the proportional contribution of the induced signal in each voltage channel.These coefficients are then used to reconstruct and subtract the unwanted induced voltage component, yielding clean, symmetrized transport data. The GUI design prioritizes accessibility, allowing experimentalists with no programming experience to process their data through a point-and-click interface. Applied to real datasets from pulsed high-field measurements, the tool demonstrated excellent performance in recovering the true voltage response of materials, reducing up/down-sweep discrepancies to within noise levels. By removing the inductive artifact, the program clarifies transport signatures, improves interpretability, and enables consistent analysis across datasets.This tool significantly enhances the workflow efficiency and measurement fidelity for condensed matter researchers utilizing pulsed field environments.

4:15pm **PCSI-SuA-10 Enhanced-Entropy Phases in Geometrically Frustrated Pyrochlore Magnets*, Prakash Timsina,*** *Ludi Miao,* New Mexico State University

Frustrated magnets host unconventional states stabilized by degeneracy and entropy, from spin ice [1] to quantum spin liquids [2] and pyrochlore oxides [3]. Pyrochlore iridates $R_2Ir_2O_7$ (R = Dy, Ho) provide a platform with tunable *d-f* exchange interactions and multiple frustrated phases [3,4]. In these systems, competing interactions suppress long-range order, yielding emergent quasiparticles such as magnetic monopoles [1].

Using Monte Carlo simulations, we map the thermodynamic phase diagram, identifying the 2-in–2-out (2I2O) spin ice, fragmented 3-in–1-out/1-in–3-out (3I1O/1I3O) [4], and all-in–all-out (AIAO) ground states [5]. In this talk, we will investigate the two finite-temperature enhanced-entropy (EE) phases near phase boundaries, characterized by high entropy, strong susceptibility, and mixed spin configurations. These phases are found to be stabilized by entropy-driven free-energy minimization, with distinct behavior of specific heat capacity decoupling from susceptibility serving as key signatures [5] (Fig. 1 in PDF). These EE states define a new class of entropy-stabilized magnetic phases, underscoring the role of frustration in finite-temperature correlated states and offering pathways for entropy-based material design.

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PCSI

Room Ballroom South - Session PCSI-SuE1

Plenary Session

Moderator: Alex Demkov, The University of Texas

7:30pm **PCSI-SuE1-1 Decoding Atomic Landscapes: Integrating Electronic Structure Theory and High-Resolution Atomic Force Microscopy***, James Chelikowsky,* University of Texas at Austin **INVITED**

Atomic force microscopy (AFM) is a transformative tool for probing matter at the atomic scale. Recent advances in high-resolution AFM (HR-AFM), especially with CO-functionalized tips, have enabled direct visualization of individual bonds and orbital features within single molecules, offering new insights into molecular structure and reactivity. These capabilities are crucial for investigating complex organic and inorganic species and surfaces.

HR-AFM leverages frequency-modulation techniques and hybrid approaches with scanning tunneling microscopy (STM) to achieve submolecular resolution. Tip functionalization enhances image contrast and sensitivity to electronic states, while theoretical frameworks—such as virtual tip models, density functional theory, frozen density embedding, and tip tilting corrections—enable quantitative interpretation of tip–sample interactions.

Our work with HR-AFM has enabled identification of bond orders, functional groups, heteroatoms, and orbital fingerprints in single molecules, as well as characterization of hydrocarbons and complex materials. Notably, we have visualized the reconstructed Si(111)-(7×7) surface, revealing atomic-scale features (see Fig.) and validating theoretical models of surface symmetry disruption [1]. These studies underscore the power of HR-AFM for resolving electronic and structural properties at the atomic level.

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PCSI

Room Ballroom South - Session PCSI-SuE2

Novel Epitaxy

Moderator: Roman Engel-Herbert, Paul-Drude Institute for Solid State Electronics

8:10pm **PCSI-SuE2-9 UPGRADED: Remote Epitaxial Frustration***, Jason Kawasaki,* University of Wisconsin Madison

Remote epitaxy promises to circumvent the lattice and chemical mismatch challenges of conventional epitaxy, to enable low defect density and chemically abrupt heterostructures of dissimilar materials. However, definitive experimental evidence for a true ``remote'' mechanisms remains elusive because most observations can be explained by alternative pinhole or van der Waals mechanisms, which are often macroscopically indistinguishable from a true ``remote'' mechanism. Here, using GdAuGe films grown on graphene/SiC (0001), we present two long-range signatures of a remote mechanism that cannot be explained by the leading alternatives: (1) a two atomic layer thick disordered interlayer at the GdAuGe/graphene interface and (2) a new $30\degree$ rotated epitaxial relationship between GdAuGe film and SiC substrate. Density functional theory calculations suggest that these signatures arise from remote epitaxial ``frustration,'' i.e. a competition between epitaxy of the GdAuGe film to the screened remote potential of the substrate (φ_{sub}), versus direct epitaxy to graphene (φ_{gr}) and to the long-range graphene-induced surface reconstruction (φ_{rec}). Our results highlight the importance of considering the multiple contributions to the total lattice potential above graphene-covered surfaces, rather than an exclusive focus on φ_{sub}. Moreover, tuning the relative magnitude and periodicities of φ_{gr}, φ_{sub}, and φ_{rec} provides new opportunities to (1) control short- and medium-range ordering of films stabilized at graphene-covered interfaces, towards the discovery of new glasses and quasicrystals, and (2) direct synthesis of rotated moire heterostructures for tuning magnetism and correlated phases

PCSI

Room Ballroom South - Session PCSI-MoM1

Group-IV Alloy Semiconductors

Moderator: Stefan Zollner, New Mexico State University

8:30am **PCSI-MoM1-1 Crystal Growth and Interface Engineering of Sn-related Group-Iv Alloy Semiconductor for Device Applications**, ***Osamu Nakatsuka***, *Masashi Kurosawa, Shigehisa Shibayama, Mitsuo Sakashita,* Nagoya University, Japan **INVITED**

Sn-related group-IV alloy semiconductors, GeSn and GeSiSn have much attracted on those unique material properties; an indirect-direct transition, a high carrier mobility, a good responsivity for near- and mid-infrared lights, a low growth temperature, a low thermal conductivity, etc. Also, the heterostructures of those alloy semiconductors realize rich energy band engineering for not only the band gap but also the band offsets like group-III-V compound semiconductors. These characters promise improved and/or superior electronic, optoelectronic, andthermoelectric device applications integrated on Si large scale integrated circuit platform.

We have developed the crystal growth technology of epitaxial and polycrystalline Sn-related group-IV alloy semiconductor thin films for device applications. There are some difficulties of the crystal growth of GeSn thin films; the low thermal-equilibrium solid solubility of Sn in Ge as low as 1%, also we have to take care for dislocations and defects with the strain relaxation on Si substrate and the low growth temperature. We need to establish the engineering technology of crystal growth and heterostructure formation with GeSn and GeSiSn to control the electrical properties. Recently, we achieved the thin film growth of a GeSn epitaxial layer with an ultra-high-Sn content over 50%. A key point for realizing such a high Sn content is the lattice-constant engineering of substrate for epitaxial growth. We used a large-lattice-constant substrate of GaSb whose lattice matches to that of $Ge_{0.48}Sn_{0.52}$ to suppress the strain between epitaxial layer and substrate.

We also achieved the heteroepitaxial growth of GeSn/GeSiSn multi layers for providing a double barrier structure. Those realize the carrier confinement structures at the valence and conduction band edges. We demonstrated its effectiveness improving optoelectronic properties enhancing photon-electron response and recently realizing the resonant tunneling diode operating at room temperature.

The development of interface engineering technology on insulator/GeSn and metal/GeSn systems is also a key issue for high-performance devices. In our presentation, we will introduce our recent achievements in an Al_2O_3/GeO_2/GeSn structure for surface passivation[5] and low-resistance NiGe(Sn)/Sb-doped Ge(Sn) contacts for electronic and optoelectronic device applications.

9:10am **PCSI-MoM1-9 Growth Orientation Analysis of Snte Epitaxial Layers on Gaas(001) Substrates by Xrd Pole Figure Measurements**, *Yingjie Chen,* Department of Electrical Engineering and Bioscience, Waseda University, Japan*;* ***Masakazu Kobayashi****,* Waseda University, Japan

SnTe, a representative IV-VI rocksalt compound, exhibits a mirror-symmetry-protected topological crystalline insulator (TCI) phase with confirmed bulk band inversion and surface Dirac states . For the band engineering, high-quality single-domain epitaxial films are crucial. Although the GaAs(001)/ZnTe buffer system enables SnTe growth, it often shows orientation competition and twinning. Hence, x-ray diffraction (XRD) pole figure analysis was used to identify those domains and their relation to growth parameters.

SnTe films were formed on GaAs(001) by molecular beam epitaxy with ZnTe buffer layers. As a representative case, sample A was grown at with a thickness of 0.2 um. Using the X-ray diffraction (XRD) θ-2θ scan, the dominant phase of the layer aligned to the substrate surface was (001). However, this technique alone cannot fully characterize complex microstructures because it is insensitive to orientations that deviate from the substrate normal. To overcome this limitation, we further performed XRD pole-figure analysis, with measuring peaks of GaAs111, SnTe200, and SnTe222 and resolving the three-dimensional configuration. It was confirmed that (001), (011), and (111) oriented domains were included in most layers. The SnTe200 pole figure exhibits (001), (011), (111) oriented domains normal to the substrate surface.The SnTe (111) component became dominant when the SnTe buffer layer was extensively annealed. An insufficient annealing duration enhances the (022) component. These findings provide an experimental basis for fabricating high-quality, single-domain SnTe epitaxial layers and will facilitate device research based on SnTe as a TCI.

This work was supported in part by a Waseda University Grant for Special Research Projects and was partly carried out at the Joint Research Center for EnvironmentallyConscious Technologies in Materials Science at ZAIKEN, Waseda University.

9:15am **PCSI-MoM1-10 Infrared Ellipsometry from 300 K to 10 K for 30 nm α-Sn Films**, ***Jaden R. Love***, *Carlos A. Armenta, Atlantis K. Moses, Jan Hrabovsky, Stefan Zollner,* New Mexico State University*; Aaron N. Engel, Chris J. Palmstrom,* University of California at Santa Barbara

α-Sn is the low-temperature phase of tin that crystallizes in an FCC diamond-like lattice structure. MBE was used to grow 30 nm thick α-Sn films on bulk undoped single side polished InSb (100) substrates [3]. The α-Sn layer on sample AE225 was grown on an Indium rich c(8x2) reconstruction and the α-Sn layer on sample AE227 was grown on an Antimony rich c(4x4) reconstruction. It has been shown that the band occupancy of α-Sn is strongly influenced by the preparation methods [2,4].

Due to relativistic effects in heavy atoms, the Γ_7^-band maximum is negative for α-Sn.There is a degeneracy at Γ and a curvature inversion of the light hole band. The degeneracy and inversion lead the Γ_8^{+v} band to appear as a valence band and the Γ_8^{+c} band to appear as a conduction band. Consequently, intervalence band transitions are allowed from the Γ_7^-band into the Γ_8^{+v}band. The oscillator strength of this transition, $\bar{E}_0$, depends on the occupancy of each band and is influenced by changing the concentration of acceptor or donor ions in the α-Sn lattice. Growth on an Indium rich interface leads to higher concentrations of acceptors that cause the oscillator strength of the $\bar{E}_0$ transition to increase. $\bar{E}_0$ is observable using infrared spectroscopic ellipsometry and has been recorded previously at 0.41 eV [2,4].

We use temperature dependent Fourier Transform Infrared Spectroscopic Ellipsometry to measure intrinsic and n-type doped 30 nm thick α-Sn layers grown on InSb (100) substrates from 300 K to 10 K. We model the dielectric function at all temperatures using a basis spline (b-spline) polynomial. Using the oscillator strength of the $\bar{E}_0$ transition we find the integrated peak intensity after a linear background subtraction and determine the hole density at each temperature by applying the Thomas-Reiche-Kuhn f-sum rule [5]. The results for the intrinsic and n-type doped samples are compared to experimental data for 70 nm α-Sn layers on InSb and CdTe substrates collected previously by [2]. We compare the experimental results to literature values obtained by using degenerate Fermi-Dirac carrier statistics [1]. We find that the carrier density is strongly influenced by substrate preparation.

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This work was supported in part by: AFOSR (FA9550-24-1-0061), ARO (W911NF-22-2-0130), NSF (DMR-2423992), and SCALE-RH (W52P1J-22-9-3009).

9:20am **PCSI-MoM1-11 Implications for Sigesn Growth from the Surface Science of Sn on Si**, ***Caitlin McCowan***, *Evan Anderson, Ezra Bussmann,* Sandia National Laboratories*; Damien West, Yunfan Liang, Shengbai Zhang,* Rensselaer Polytechnic Institute

SiGeSn is a promising alloy for optoelectronic applications due to having a simpler path for integration into silicon semiconductor manufacturing than compound semiconductors. A direct bandgap has been predicted theoretically, but has not been definitively observed experimentally. This discrepancy is thought to result from the atoms in the lattice not forming a random alloy, but exhibiting short range order. Curiously, SiGe has the same underlying atomic- and mesoscopic-scale forces, i.e. bonding and strain, but is a random alloy. The goal of this research is to understand what is driving short range ordering in SiGeSn alloys. We collected data with scanning tunneling microscopy (STM), analyzing growth in a step-by-step fashion where sub-monolayer Sn is deposited on to a Si(100) substrate, and then annealed. Step-by-step tuning of growth and annealing variables can be analyzed *in situ* with STM.

Atomic scale analysis of the Sn:Si surface gives insight into what drives ordering of group IV alloys. Our data shows Sn deposited on Si forms 2x1 dimer chains, but, unlike Si deposited on Si, they don't pack closely together due to steric repulsion. After annealing, Sn both assembles into

islands at the surface as well as incorporates into the topmost layer of Si atoms in the substrate, but with a 3x2 periodicity (Fig 1). The change implies an interaction between the local strain inherent to the dimer rows, bonding, and steric repulsion. Sn coverage, annealing time, and annealing temperature collectively change the appearance of structures above the atomic scale – e.g. the length of the chains. Meanwhile, only the long-range periodicity of these features is dictated by the strain. Atomic positions from the experimental data will be compared to predictions from modeling.

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9:25am **PCSI-MoM1-12 Pressure-Dependent Photoluminescence of a Gesn/Sigesn Single Quantum Well at 10 K***, **Meghan Worrell,*** New Mexico State University

The 10 K photoluminescence (PL) properties of a GeSn/SiGeSn single quantum-well (SQW) heterostructure are measured as a function of hydrostatic pressure applied using a diamond anvil cell (DAC) from 0 to ~0.5 GPa. With increasing pressure, the PL peak exhibits a consistent blueshift with a clear reduction in intensity beyond ~0.5 GPa due to PL quenching. The PL peak energy increased linearly with pressure, resulting in a pressure coefficient of approximately 48 meV/GPa. By fitting the PL energy shift against strain calculated using the Murnaghan equation, the hydrostatic deformation potential is evaluated as −3.5 ± 0.1 eV. The strain in the GeSn/SiGeSn structure is evaluated using high-resolution X-ray diffraction (XRD) and reciprocal space mapping (RSM) along both (004) and (224) directions. These measurements allowed precise determination of in-plane and out-of-plane lattice constants for the quantum well, buffer, and barrier layers. Using these lattice parameters, the hydrostatic and shear strain components are calculated for each layer in the heterostructure, enabling determination of the band edge alignment as a function of strain. The results provide insights into band structure engineering in GeSn/SiGeSn QWs and demonstrate their tunable optical properties under external pressure.

9:30am **PCSI-MoM1-13 Group IV Alloy Short-Range Order and Fluctuation Effects on Quantum Electronics***, **Ezra Bussmann,*** Sandia National Laboratories **INVITED**

Recent progress with spin quantum computing and lasers in group IV (Si, Ge and Sn) alloy heterostructures revealed alloy fluctuations and correlations that have appreciable influence on materials electronic properties [1-3]. This has inspired high-fidelity studies exploring fluctuations and short-range order across group IV alloys [3-5]. Here, short-range order (SRO) denotes atomic neighborhood correlations between alloy elements site-to-site on the diamond-type crystal lattice, whereas fluctuation denotes neighborhood statistical variations from mean composition. I will describe experiments to detect subtle nanosize alloy fluctuations and SRO, and theory and models to explain their origins and outsized effect on single-particle states for qubits in SiGe and electronic bands in SiGeSn. For electron spin qubits in SiGe heterostructures, alloy fluctuations modify splittings separating qubit states from other excited states, allowing state mixing and quantum leakage paths [3].In SiGeSn, SRO correlations emerge above background alloy fluctuations, and this SRO is predicted to modify electronic band parameters, electronic and thermal transport, and materials design [2]. I will describe ongoing work to measure and isolate these effects and to design and control alloy fluctuations and SRO as an electronic engineering degree-of-freedom. The talk will highlight advances around the group IV epitaxial material community, through collaborations in the *Center for Manipulation of Atomic Ordering for the Manufacture of Semiconductors* (*μATOMS*) a recently funded *Energy Frontier Research Center*, and my teams work on fluctuations affecting qubit variability in SiGe materials [5].

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PCSI

Room Ballroom South - Session PCSI-MoM2

Materials for QIS

Moderator: Edward Yu, The University of Texas at Austin

11:00am **PCSI-MoM2-31 UPGRADED: Er:Si and SiC on Insulator for Quantum Information Processing***, **Sven Rogge,*** University of New South Wales, Australia

Optically active spins in solid-state systems present significant potential for a range of quantum information science applications, including their use as entanglement distribution nodes within quantum networks, single-photon sources for linear optical quantum computing, and as platforms for cluster state quantum computation. Furthermore, the inherent optical connectivity of these systems enables the implementation of low-density parity check (LDPC) error correction codes. Among these platforms, erbium ions implanted in silicon and silicon carbide are particularly promising due to their superior optical and electron spin coherence characteristics, erbium's emission compatibility with the Telecom C band, and the advanced state of silicon nanofabrication technology. In this work, we report on erbium sites in silicon that simultaneously exhibit extended optical coherence and long electron spin lifetimes. Specifically, we observed spin coherence times of 1 ms in nuclear spin-free silicon crystals. The measured homogeneous linewidths were below 100 kHz, with inhomogeneous broadening approaching 100 MHz [1]. Spectral hole burning and optically detected magnetic resonance techniques were employed to examine both the homogeneous linewidth and spin coherence properties. The demonstration of long spin coherence times and narrow optical linewidths in multiple sites underscores the exceptional suitability of erbium in 28Si for future quantum information and communication technologies, including single-photon frequency multiplexing schemes. Further discussions address the integration of these systems into silicon-on-insulator nanophotonic devices as well as thin-film 4H-SiC-on-insulator (SiCOI) devices. In silicon carbide, we observed an inhomogeneous broadening of 6.22 GHz and homogeneous linewidths as narrow as 440 kHz from a weak ensemble of emitters [2]. Site-selective spectroscopy identified that Er ions primarily occupy two distinct lattice sites in 4H-SiCOI. Additionally, we characterized the optical lifetimes and magneto-optical properties of these narrowband transitions. Collectively, these findings position Er-doped SiCOI as a highly promising solid-state platform for integrated, on-chip quantum information processing applications.

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11:20am **PCSI-MoM2-35 Engineering Telecom-Wavelength Quantum Dots via Epitaxial Growth on Inp and Gaas for Single-Photon Applications***, **Jesus Marquez,*** Sandia National Laboratories

This work explores two promising approaches for fabricating single-photon emitters operating at telecom wavelengths (1.3–1.55 μm), using epitaxially grown quantum dots (QDs). The first approach involves the growth of InAs nanostructures on InP substrates, producing a mix of quantum dots and dashes. On standard InP (100) substrates, growth proceeds via a modified Stranski–Krastanov (SK) mechanism, where a thick, planar wetting layer forms prior to 3D island nucleation. These elongated dashes, preferentially aligned along the (1-10) direction, exhibit limited three-dimensional confinement, behaving more like quantum wells. In contrast, growth on (311)B-oriented InP yields discrete QDs with strong single-dot emission characteristics.[1]

The second approach leverages the GaSb/GaAs material system to realize both coherently strained SK-mode QDs and strain-relaxed islands, the latter mediated by interfacial misfit dislocation arrays. Despite its promise, this system faces challenges due to likely type-II band alignment and the complexity introduced by GaSb/GaAs interdiffusion during capping.

Growth experiments are conducted using a solid-source VG V80 MBE reactor. InAs QDs are deposited on n-doped InP (001) and (311B) substrates with $In_{0.53}Ga_{0.47}As$ buffer layers, while GaSb QDs are grown on semi-insulating GaAs (001) with GaAs buffer layers. Substrate desorption, growth temperatures, and layer thicknesses are carefully optimized.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

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11:30am **PCSI-MoM2-37 Revisiting Surface Conditions of H/Si(111) after Wet-Chemical Treatment through Different SPM Modes**, ***Ayumi Takahashi***, *Az Zahrah Fitriana Syafira, Naoko Momono, Marimi Kuwano, Kouji Inagaki, Kenta Arima,* The University of Osaka, Japan

High-performance solution processing is essential for next-generation electronic and optical devices, and Scanning Probe Microscopy (SPM) enables atomic-scale evaluation. This report aims to characterize wet-treated Si(111) surfaces in detail using multiple SPM modes.

Si(111) surfaces were treated by anisotropic etching in NH_4F [1]. These surfaces were first imaged in air by conventional amplitude-modulated Atomic Force Microscopy (AFM). Figure 1(a) shows a familiar step/terrace structure. The same surface was then examined by noncontact AFM (nc-AFM) and Scanning Tunneling Microscopy (STM). The nc-AFM/STM hybrid system was operated at room temperature under ultrahigh-vacuum conditions of 10^{-8}–10^{-7} Pa. For nc-AFM, the oscillation amplitude and frequency shift were set to 1.0 nm and −1.0 Hz, respectively, and for STM, the sample bias and tunneling current were −2.0 V and 0.6 pA. It is evident that the nc-AFM image in Fig. 1(b) resolves smaller particles or adsorbates with much higher resolution than Fig. 1(a). More importantly, these small particles visible in Fig. 1(b) are absent in the STM image in Fig. 1(c). A subsequent nc-AFM scan of the same area after acquiring Fig. 1(c) reproduced the result in Fig. 1(b), confirming that Fig. 1(c) does not arise from probe-induced manipulation of adsorbates but rather from the different imaging mechanisms of nc-AFM and STM.

The X-ray Photoelectron Spectroscopy (XPS) spectrum in Fig. 2, obtained with the same sample, reveals carbon and oxygen signals in addition to Si. This indicates that the small particles in the nc-AFM image in Fig. 1(b) likely correspond to organic contaminants or water molecules with low conductivity. Their probable origin is sample preparation in air, ranging from the NH_4F treatment itself to the subsequent transfer process. In contrast, the fine particles observed in the STM image in Fig. 1(c) are attributed to Si dissolved in NH_4F and redeposited on the surface. These results demonstrate that the combination of nc-AFM and STM provides complementary insights into the molecular-level distribution of adsorbates, which will be valuable for advancing solution-based processes such as wet cleaning.

11:35am **PCSI-MoM2-38 Characterizing Point Defect Damage from Proton Irradiation in Narrow Bandgap Materials**, ***Evan M. Anderson***, Sandia National Laboratories; *Rigo A. Carrasco, Christopher P. Hains, Alexander T. Newell,* Air Force Research Laboratory; *Marcos Calva, Austin Shipley,* New Mexico State University; *Devika Mehta,* Sandia National Laboratories; *Preston T. Webster,* Air Force Research Laboratory; *Aaron J. Muhowski, Lilian K. Casias, John M. Cain, Victor J. Patel,* Sandia National Laboratories; *Boris Kiefer,* New Mexico State University; *Christian P. Morath,* Air Force Research Laboratory; *Eric A. Shaner, Peter A. Schultz,* Sandia National Laboratories

Narrow bandgap semiconductor heterostructures are used for a wide variety of applications, including infrared sensing in space. However, sensor performance can suffer in the space environment through the formation of point defects caused by ion irradiation. This degradation is often studied to derive an empirical damage factor characterizing the decline in performance as a function of dose for a given epitaxial detector stack. A key metric in evaluating these detector materials is the minority carrier lifetime, which directly corresponds to leakage current and detectivity. While this approach is crucial for evaluating detectors and predicting their useable service life, it does not identify the precise defect trap states that are created and decrease minority carrier lifetime. Thus, identifying the atomic scale defects and their energy levels that are present both from materials growth are critical for characterizing and improving the performance of infrared detectors.Identifying defects in narrow bandgap materials presents a distinct challenge: all defects are shallow and are difficult to resolve from band edges. Further, these defects are active even at cryogenic temperatures. Thus, we take a multifaceted approach combining theory and experiment, focusing on InAs as a model system to build a foundation for understanding more complex alloys and heterostructures. We use electronic device measurements including deep level transient spectroscopy, and material characterization such as time-resolved microwave reflectance and time-resolved photoluminescence to measure minority carrier lifetime, and compare these results to candidate point defects predicted by ab initio calculations. This approach allows us to resolve the ambiguities in experimental data that can only quantify defect activation energies without knowledge of their atomic structure, while sifting out the variety of defects that might be predicted to be stable but that do not correspond to experiments.SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

11:40am **PCSI-MoM2-39 High-Frequency Shunt Behavior in Granular Metals**, ***Matthew Landi***, *Michael McGarry, Simeon Gilbert, Jacob Eisbrenner, Michael Siegal, Laura Biedermann,* Sandia National Laboratories, USA

Granular metals (GMs) are a class of disordered materials comprising metal nanoparticles (NPs) dispersed within an insulating matrix. As a result of theirnanostructure, GMs exhibit complementary resistive tunneling and capacitive charge transport properties. These parallel processes give GM's a high-pass filter like behavior[1], such that the conductivity displays a power-law behavior as a function of the drive frequency. Due to their high breakdown electric-field strength and high-pass nature, GMsmake for attractive shunt devices for high-power, high-frequency applications In this work, GMs are grown via radiofrequency co-sputtering using molybdenum (Mo)and silicon nitride (Si3N4) targets[2]. We show that the Mo NP size, density, and spacing is controllable via the growth conditions and post-growth annealing recipes (Fig. 1A).Manipulating the intercalation of the Mo NPs enables great control of the GM electrical properties. The effect of Mo metal fraction and annealing temperature on GM conductionis investigated via temperature-controlled impedance spectroscopy (Fig. 1B, C). Here, a universal power-law distribution in the conductivity is observed, characteristic ofmany disordered material systems [3,4]. These GMs exhibit conductivity swings on the order of sMHz/sDC of 106. Vertical shunt devices with 0.5 cm2 GM active area arefabricated on antimony-doped conductive silicon (N-type). These films shunt 25 Amps at 2.25 MV/cm (Fig. 1D). This systematic investigation and fabricationof functional GM films serves to bridge the gap between the processing, structure, and electrical properties of GMs and more generalized disordered systems.[1] H. Bakkali, M. Dominguez, X. Batlle and A. Labarta, Sci. Rep. 6, 29676 (2016)[2] M. McGarry, et al. J. Appl. Phys. 136, 055101 (2024)[3] A. Jonscher, Thin Solid Films 36 (1), 1-20 (1976)[4] L. Merle, A. Delpoux, A. Mlayah and J. Grisolia, J. Appl. Phys. 132 (1), 015107 (2022)

11:45am **PCSI-MoM2-40 Enhancement of Superconductivity in Cryogenically Grown Ultra Thin Al Films**, ***Teun van Schijndel***, *Yu Wu, Wilson Yánez-Parreño, Tawshia Chowdhury, Julian Choi, Christopher Palmstrøm,* UC Santa Barbara

Superconductivity in thin films can deviate significantly from bulk behavior, especially as dimensionality and disorder come into play. This is particularly true for aluminum, where critical temperature (T_C) and film morphology are highly sensitive to thickness and growth conditions. Here, we present an *in-situ* scanning tunneling microscopy (STM) study, performed at 78 K, of Al thin films grown on atomically clean Si(111) substrates by molecular beam epitaxy at cryogenic temperatures down to 6 K. The morphology is characterized across a wide range of coverages, from sub-monolayer up to 20 monolayers (ML). Cryogenic growth results in oriented hexagonal islands that begin to coalesce into a continuous film around 5 ML, with a typical roughness of a few monolayers. This roughness is constant up to 20 ML. Upon annealing to room temperature, the surface becomes nearly atomically smooth, though grain boundaries remain visible in STM. In contrast, room temperature growth produces significantly rougher films with large, disconnected islands of varying shape and orientation. We also investigated the superconducting properties of cryogenically grown films after exposure to atmospheric conditions, as required for ex-situ transport measurements. To stabilize the films, we used different post-growth treatments, including low temperature capping, cold oxidation, and room temperature oxidation. The films show critical temperatures approaching 3 K and critical fields above 5 T, which are significantly above the bulk value of 1.2 K.

11:50am **PCSI-MoM2-41 Imaging Field-Induced Metastable DX Center Formation in Near-Surface Region of *n*-type InAs by Scanning Tunneling Microscopy***, Kiyoshi Kanisawa,*** Basic Research Laboratories, NTT, Inc., Japan

Control of semiconductor nanostructures becomes more important to achieve the further device miniaturization [1]. Especially, critical significance of charge and spin states becomes evident at atomic-scale precision [2]. Donor-related defect-complex, DX center, in III-V semiconductors is one of lattice defects. Charge states of this defect as well as the bistable switching on the long lifetime were studied for Si-doped *n*-GaAs [3]. In the case of InAs, static transition of acceptor charge states in Mn-doped *p*-InAs is only reported [4].

In this presentation, the DX center in the near-surface region of *n*-type InAs is demonstrated as a quasi-equilibrated metastable state by using the scanning tunneling microscope (STM). After obtaining the cleaved (110) surface of sulfur-doped *n*-InAs (N_S : 4×10^{17} cm^{-3}) in ultra-high vacuum, the sample was transferred to the STM stage kept at 77 K. First, it is found that donor charge states showed striking dependence on the STM tip at the same scan condition. This suggests that the degree of the tip-induced band bending plays the crucial role of the charge state determination. Second, it is found that electrons tunneled from the STM tip cause an impact-ionization by the tip-induced electric field acceleration at the sample bias voltage $V > 0$ (tip is neutral). When the electric field exceeds the Avalanche breakdown field ($\sim 8 \times 10^{-5}$ V/nm) [5], such hot electrons cause the impact-ionization. Generated secondary electrons are spread by radially diverging tip-induced field. At this non-equilibrium situation, the electron quasi-Fermi level becomes locally dominant to charge states of donor-related defects [6] beneath the tip. This quasi-Fermi level effect is detected as the bias voltage dependent topography. No evident bistable switching among charge states is imaged. These suggest that the imaged DX center in the *n*-InAs is a quasi-equilibrated metastable state available at the non-equilibrium condition and the lifetime of the captured electron by such DX center is expected much shorter than that of *n*-GaAs.

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11:55am **PCSI-MoM2-42 Giant Chiral Magnetoelectric Oscillations in a van der Waals Multiferroic***, **Xinyue Peng**, Frank Gao,* UT Austin*; Xinle Cheng, Emil Viñas Boström,* Max Planck Institute for the Structure and Dynamics of Matter, Germany*; Dongseob Kim,* UT Austin*; Ravish Jain,* Academia Sinica, Taiwan*; Deepak Vishnu,* National Tsing Hua University, Taiwan*; Kalaivanan Raju,* Academia Sinica, Taiwan*; Raman Sankar,* Academia sinica, Taiwan*; Shang-Fan Lee,* Academia Sinica, Taiwan*; Michael Sentef,* Max Planck Institute for the Structure and Dynamics of Matter, Germany*; Takashi Kurumaji,* Caltech*; Xiaoqin Li,* UT Austin*; Peizhe Tang, Angel Rubio,* Max Planck Institute for the Structure and Dynamics of Matter, Germany*; Edoardo Baldini,* UT Austin

Helical spin structures are expressions of magnetically induced chirality, entangling the dipolar and magnetic orders in materials. The recent discovery of helical van der Waals multiferroics down to the ultrathin limit raises prospects of large chiral magnetoelectric correlations in two dimensions. However, the exact nature and magnitude of these couplings have remained unknown so far. Here we perform a precision measurement of the dynamical magnetoelectric coupling for an enantiopure domain in an exfoliated van der Waals multiferroic. We evaluate this interaction in resonance with a collective electromagnon mode, capturing the impact of its oscillations on the dipolar and magnetic orders of the material with a suite of ultrafast optical probes. Our data show a giant natural optical activity at terahertz frequencies, characterized by quadrature modulations between the electric polarization and magnetization components. First-principles calculations further show that these chiral couplings originate from the synergy between the non-collinear spin texture and relativistic spin–orbit interactions, resulting in substantial enhancements over lattice-mediated effects. Our findings highlight the potential for intertwined orders to enable unique functionalities in the two-dimensional limit and pave the way for the development of van der Waals magnetoelectric devices operating at terahertz speeds.

Reference:

Gao, F.Y., Peng, X., Cheng, X. *et al.* Giant chiral magnetoelectric oscillations in a van der Waals multiferroic. *Nature*632, 273–279 (2024). https://doi.org/10.1038/s41586-024-07678-5

PCSI

Room Ballroom South - Session PCSI-MoA1

Layered Magnetism

Moderator: Christopher Palmstrøm, University of California, Santa Barbara

2:00pm **PCSI-MoA1-1 Dielectric Tensor, Magnetic Anisotropies and Coupled Excitations in Layered Magnetic Semiconductors CrSBr**, ***Ursula Wurstbauer,*** University of Münster, Germany **INVITED**

Two-dimensional materials exhibit unique properties due to their atomically thin structure and weak van der Waals (vdW) coupling between layers resulting in layer dependent properties. As in the case of the layered magnetic semiconductor CrSBr, individual layers are ferromagnetically ordered below the Neel temperature (T_N»132K), while adjacent layers are coupled antiferromagnetically. Due to the highly anisotropic electronic bands in CrSBr, electronic and excitonic states at the fundamental band-gap behave quasi-one-dimensional [1]. Moreover, the resulting excitonic transitions are highly sensitive to the collective spin order. Below the critical temperature, an external magnetic field applied along the magnetic hard directions drives the system from the antiferromagnetic into a ferromagnetically ordered state causing a quadratic red-shift of the exciton energies theoretically explained by spin-allowed charge transfer changing the composition and nature of excitons [2]. By a combination of magneto-reflectance, magneto-photoluminescence and magneto resonant inelastic light scattering (RILS) experiments, we study strong coupling between charge, lattice and spin degrees of freedom as well as their changes when interfaced to other 2D magnetic semiconductors from the transition metal phosphor trisulfide group with different magnetic anisotropies.

The strong light matter interaction in thin CrSBr film is highly tunable by layer number and magnetic polarization. To develop a better understanding, we access the materials dielectric tensor in the paramagnetic and ferromagnetic phase by variable-temperature spectroscopic imaging ellipsometry. In agreement with theory, we extract highly anisotropic dielectric functions along the crystallographic main axes with strong excitonic resonances particularly in the plane [4].

We acknowledge the fruitful collaboration with Florian Dirnberger, Julian Klein, Zdeněk Sofer, Marie-Christin Heißenbüttel, Thorsten Deilmann and Michael Rohlfing.

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2:40pm **PCSI-MoA1-9 Magneto-Optical Studies of Layered Antiferromagnet $CrPS_4$**, ***Jongchan Kim,*** Seoul National University, South Korea*; Kenji Watanabe, Takashi Taniguchi,* NIMS (National Institute for Materials Science), Japan*; Je-Geun Park, Jieun Lee,* Seoul National University, South Korea

Two-dimensional magnetic materials have recently attracted significant attention as promising platforms for studying spin-based devices such as spin filters or valves and investigating exotic spin-dependent phenomena such as the realization of magnetic skyrmions. However, micrometer-scale dimensions of these materials make their direct magnetic characterization challenging. Conventional bulk measurement techniques are often insufficient, therefore, approaches through transport measurements or optical probes must be employed. In this work, we investigate thin-layers of antiferromagnetic semiconductor $CrPS_4$, which is an A-type antiferromagnet in its bulk form, and explore its spin properties through magneto-optical effects and polarization-resolved photoluminescence (PL) measurements.

The few-layer flakes of $CrPS_4$ investigated in our work are obtained by mechanical exfoliation from bulk crystals which are subsequently capped with hBN. For probing the spin polarization, we measured the degree of circular polarization of PL emission from $CrPS_4$ in Faraday geometry and confirm the out-of-plane spin orientation which is further supported by the magnetic circular dichroism (MCD) measurements. We further extend our study to the Voigt geometry, performing both MCD and circularly polarized PL measurements to track the evolution of spin orientation under in-plane magnetic fields. Taken together, these optical spectroscopic results demonstrate the potential of two-dimensional antiferromagnets as versatile platforms for exploring spin physics in van der Waals platforms and advancing next-generation spin-based technologies.

2:45pm **PCSI-MoA1-10 UPGRADED: Van der Waals Antiferromagnets $Co_{1/3}NbS_2$ and $Co_{1/3}TaS_2$: Topological Magneto-Optics & Tunable Chiral/Nematic Phases**, ***Scott Crooker,*** National High Magnetic Field Laboratory

The family of intercalated niobium and tantalum dichalcogenides, $M_{1/3}NbS_2$ and $M_{1/3}TaS_2$ (where M= V, Cr, Mn, Fe, Co, Ni), are van der Waals materials hosting layers of spins on 2D triangular lattices -- an archetypal frustrated network that can lead to a rich variety of complex magnetic states.$Co_{1/3}NbS_2$ and $Co_{1/3}TaS_2$ are antiferromagnets (AFMs) that exhibit giant spontaneous Hall conductivity despite vanishing net magnetization [1], suggesting nontrivial AFM order and potential for AFM spintronics. Recent neutron diffraction studies point to a non-coplanar “tetrahedral” triple-**Q** AFM order with scalar spin chirality [1]. In contrast to conventional collinear AFM order, this (and certain other) complex AFM spin configurations can allow for off-diagonal Hall conductivity, σ_{xy}, which in turn generates anomalous and topological Hall effects in transport studies.

Crucially, $\sigma_{xy}(\omega)$ is frequency-dependent, and at optical frequencies it generates Kerr rotation and magnetic circular dichroism (MCD).Thus, the full power of optics, including imaging and spectroscopy, can be applied to study complex AFM orders in $Co_{1/3}NbS_2$ and $Co_{1/3}TaS_2$.Here we show [2,3], using light spanning infrared-ultraviolet (1-3 eV), that MCD is a powerful and incisive probe of chiral triple-**Q** AFM order. Measurements at different photon energies are compared with DFT calculations. Scanning MCD microscopy is used to directly image (and also write) chiral 3**Q** domains. In $Co_{1/3}TaS_2$, linear dichroism studies also reveal three-state (Z_3) nematicity arising from a single-**Q** stripe phase, as well as phases where chirality *and* nematicity coexist [3]. A theoretical analysis based on a *continuous multi-**Q** manifold* captures the emergence of these distinct magnetic phases, resulting from the interplay between four-spin interactions and weak magnetic anisotropy. Our findings establish $Co_{1/3}TaS_2$ as a rare platform hosting diverse multi-**Q** states with distinct combinations of spin chirality and nematicity).

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3:10pm **PCSI-MoA1-15 Highly Efficient Interlayer Exciton Microcavity Laser in Free-standing 2D Heterostructures**, ***Yeeun Cho,*** Seoul National University, South Korea*; Kenji Watanabe,* Research Center for Electronic and Optical Materials, National Institute for Materials Science, Japan*; Takashi Taniguchi,* Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan*; Jieun Lee,* Seoul National University, South Korea

Monolayer transition metal dichalcogenides (TMDs) and their heterostructures offer a versatile platform for photonics owing to their atomic thickness and strong excitonic interactions. Interlayer excitons (IXs) in heterobilayers possess long lifetimes and tunable emission energiesleading to various interesting phenomena, yet their weak oscillator strength limits emission intensities and lasing behaviors.In this work, we report efficient IX lasing from a $MoSe_2/WSe_2$ heterobilayer through integrationwith a free-standing silica microsphere cavity. The suspended geometry enhances IX emission by more than an order of magnitude relative to supported regions and enables efficientcoupling to high-*Q* cavity(*Q* ~2600). A lasing threshold as low as 75 nW is observed, as confirmed by the superlinear emissionkinkand linewidth narrowingin the power dependence measurements.The lasing threshold of the suspended sample is reduced by more than ten times compared to thesupported samples, consistent with the measuredIX lifetimes.These findings establish free-standing van der Waals heterostructures integrated with microcavities as compact and low-powerconsumptioncoherent light sources for quantum photonicsapplications.

3:15pm **PCSI-MoA1-16 Strain-Programmable Exciton Diffusion in Moiré Heterostructures**, ***Chiho Song,*** Seoul National University, South Korea*; Chiranjit Mondal,* Seoul National University, South Korea, India*; Jaebin Lee,* Seoul National University, South Korea*; Kenji Watanabe, Takashi Taniguchi,* NIMS (National Institute for Materials Science), Japan*; Bohm Jung Yang, Jieun Lee,* Seoul National University, South Korea

Moiré superlattices in van der Waals heterostructures based on two-dimensional materials have recently gained significant attention as an intriguing platform for exploring strongly correlated electronic states and

engineering novel excitonic properties. Such superlattices have been generally created and tuned either by lattice constant mismatch or layer twisting. However, strain is also a powerful tool for tuning the moiré superlattices, which yields fascinating features distinct from the twisted cases due to the C_3 rotational symmetry breaking. Herein, we experimentally and theoretically investigate the optical properties of interlayer excitons (IXs) generated in strain-induced $MoSe_2$-WSe_2 heterobilayers.

In our experiment, we fabricated vertically stacked MoSe2-WSe2 heterobilayers in which uniaxial strain is applied to a single constituent layer. Due to the type-II band alignment, the heterobilayer exhibits long-lived IXs with electrons and holes spatially separated in opposite layers. We probe the strain effect on the IX emission polarization and diffusion over the stacked region which shows peculiar coupling of the excitonic behavior with the strain-induced moiré potentials. Firstly, we found the linearly polarized IX emission resulting from the C3 rotational symmetry breaking of the moiré potential over a wide spatial area. Secondly, through spatially resolved IX diffusion measurements, we found that IXs diffuse preferentially along the applied strain direction over several micron scales. Our experimental observations are also consistent with the density functional theory (DFT) calculation results of the strain-induced moiré potential landscapes.

PCSI

Room Ballroom South - Session PCSI-MoA2

Wide Band Gap Semiconductor & DUV Lithography

Moderator: Jason Kawasaki, University of Wisconsin - Madison

4:20pm **PCSI-MoA2-29 Polarization Birefringence and Surface Roughness of XeLiF + Al Mirrors**, ***Nathan Skousen,*** Brigham Young University*; Sarah Loewecke,* Fordham University*; James Hilfiker,* J.A. Woollam Co., Inc.*; Luis Rodriguez de Marcos,* Catholic University of America, Spain

A new deposition method developed by Goddard Space Flight Center fluorinates the surfaces of freshly evaporated Al mirrors by exposure to XeF2. This produces an ultrathin film of aluminum fluoride which is thought to conformally coat the aluminum. This is followed by an evaporated LiF coating to create a broadband, relatively stable mirror which is termed Al+XeLiF. This in-situ, room-temperature process produces mirrors with noteworthy environmental stability and high reflectance over a broad spectral range from the FUV to the IR, including the desirable, but hard to achieve, 100 to 115 nm range. NASA may use this approach to prepare mirrors and grating coatings for the future Habitable Worlds Observatory. To accomplish its primary mission of imaging and characterizing potentially habitable exoplanets the HWO requires total extinction of the light from an exoplanet's star to capture the light of dim exoplanets without contaminating starlight. When used with an internal coronograph, however, surface roughness and polarization effects from the telescope mirrors could result in starlight leaking into the coronograph's dark pit preventing clear detection and characterization of Earth-size planets in a star's habitable zone. We studied retardance and diattenuation using variable-angle, spectroscopic ellipsometry (VASE) to better understand these effects on lithium-fluoride-coated aluminum mirrors exposed to different temperature/humidity environments.

The physical evolution of roughness on deposited fluoride surfaces is noteworthy. Fluorides, particularly LiF, are observed to roughen in moist air even at relatively low humidity. Water condenses out of the air in any small defects due to Laplace pressure. Condensed water will attack the film. Then, in an Oswald ripening-type process, larger crystals form at the expense of nanometer size crystals. This creates defects even more favorable for the condensation of moisture and the eventual destruction of the film.

4:25pm **PCSI-MoA2-30 Beyond Isotropy of Cubic Crystals**, ***Beáta Hroncová,*** Masaryk University, Czechia*; Subiao Bian, Oriol Arteaga,* Universitat de Barcelona, Spain*; Razvigor Ossikovski,* Institut Polytechnique de Paris, France

The dielectric response of cubic crystals, like Si, Ge, GaAs, InSb, and CaF_2, is commonly assumed to be isotropic. This assumption stems from the fact that, at optical frequencies, the wavelength of light is much larger than characteristic distances inside the crystal (usually of the order of interatomic distances), $a/\lambda<<1$. Within this limit, the macroscopic material response is local. This description breaks down mainly in the spectral region near excitations, where the refractive index increases and the ratio a/λ becomes non-negligible. Keeping non-local terms in the dielectric tensor explains the weak anisotropy observed in cubic crystals [1]. The intrinsic birefringence has caused many problems in the semiconductor industry, where cubic crystals are widely used as substrates for layer growth. Substrate anisotropy can make optical characterization of the layers challenging. Another example is the failure of 157nm lithography, where the crystals used for UV laser optics, CaF_2 and BaF_2, exhibit unacceptably large birefringence [2].

In this work, we utilize high-sensitivity Mueller matrix polarimetry to measure the weak anisotropy of cubic crystals. This approach has recently been shown to work well for reflection measurements on silicon [3]. We also present our transmission experimental results that show intrinsic birefringence of Si and CaF_2. In addition, we demonstrate the directional dependence of the intrinsic birefringence by examining crystals with different surface orientations. Rotational symmetries of the crystal axes are clearly visible (Fig. 1), indicating that the measured birefringence is intrinsic and not induced, e.g. by strain.

4:30pm **PCSI-MoA2-31 Investigating the Dust Mitigation Abilities of Dissociative Degradation**, ***Kira Sand,*** Brigham Young University

Particulate contamination requires dust mitigation techniques to provide low-scatter surfaces on sensitive instrumentation in space. We have previously shown that poly(olefin sulfone)s photodegrade in spacelike conditions: in vacuum and with UV light exposure. We now demonstrate that photodegradable polymers can reduce dust accumulation on optical surfaces for space applications. Our research shows that dissociative degradation of poly(olefin sulfone)s significantly decreased the number of dust particles on a dust-coated surface.

Our findings show a viable way to mitigate the collection of extraterrestrial dust on optical surfaces in space, enabling passive removal of particulate contamination without any direct human intervention.

4:40pm **PCSI-MoA2-33 Development of UV-C light Source in 180-190 nm Spectral Range using Rocksalt-structured MgZnO Alloys**, ***Takeyoshi Onuma,*** 2665-1 Nakano, Hachioji, Japan*; Kotaro Ogawa,* Kogakuin University, Japan*; Yuichi Ota,* Toyama Prefectural University, Japan*; Kentaro Kaneko,* Ritsumeikan University, Japan*; Tomohiro Yamaguchi,* Kogakuin University, Japan*; Shizuo Fujita,* Kyoto University, Japan*; Tohru Honda,* Kogakuin University, Japan **INVITED**

The Minamata Convention on Mercury is advancing the regulation of mercury products. However, low-pressure mercury lamp is exempted from the regulation. The 185 nm emission is widely utilized as a light source for oxygen dissociation, ozone generation, and OH radical production in water treatment, while the 254 nm emission is widely used for UV sterilization. Although AlGaN-based deep UV LEDs are becoming promising alternative to the 254 nm emission, almost no effort has been made to replace the 185 nm emission.Behind the background, we have studied rocksalt (RS)-structured MgZnO alloys as candidate materials for UV-C emitters in 180-190 nm spectral range. Our group has reported growth of atomically-flat single crystalline RS-MgZnO films on MgO (100) substrates by using the mist chemical vapor deposition (mist CVD) method [1-3]. Observations of deep UV cathodoluminescence (CL) have been reported [1–6]. Post-growth slow-cooling process was used to improve the crystallinity and emission properties [7]. A near-band-edge emission was eventually achieved in the 187–223 nm spectral range at 300 K. Our group also succeeded in growing RS-MgZnO polycrystalline films on quartz glass substrates using the mist CVD [8]. The achievement brought us a demonstration of RS-MgZnO-based UV-C lamp emitting in 190-220 nm spectral range using 146 nm line of Kr_2^* generated by dielectric barrier discharge as an excitation light source [9]. The progresses and recent achievements in growth of RS-MgZnO/MgO multiple quantum well structures will be discussed.This work was supported in part by Grants-in-Aid for Scientific Research Nos. 17H01263, 20H00246, 22K04952, 25K08495, and 25KJ2089 from MEXT, Japan and The Canon Foundation. T.O. would like to thank Prof. S. F. Chichibu and Dr. K. Shima of Tohoku University for their help with time-resolved photoluminescence measurements. The RS-MgZnO-based UV-C lamp was developed as a joint research project between ORC Manufacturing Co., Ltd. and Kogakuin University.[1] K. Kaneko *et al*., Appl. Phys. Express **9**, 111102 (2016). [2] K. Kaneko *et al*., J. Electron. Mater. **47**, 4356 (2018). [3] K. Ishii *et al*., Appl. Phys. Express **12**, 052011 (2019). [4] T. Onuma *et al*., Appl. Phys. Lett. **113**, 061903 (2018). [5] M. Ono *et al*., J. Appl. Phys. **125**, 225108 (2019). [6] T. Onuma *et al*., J. Appl. Phys. **134**, 025102 (2023). [7] K. Ogawa *et al*., Jpn. J. Appl. Phys. **63**, 02SP30 (2024). [8] W. Kosaka *et al*., Phys. Status Solidi B **259**, 2100354 (2021). [9] K. Ogawa *et al*., Appl. Phys. Express **17**, 121001 (2024).

5:20pm **PCSI-MoA2-41 Epitaxy of β-Ga2O3 on Highly-Offcut (>10°) Substrates**, ***M. Brooks Tellekamp***, *Anna Sacchi, John Mangum,* National Lab of the Rockies*; Drew Haven, David Joyce,* Luxium Solutions*; Andriy Zakutayev,* National Lab of the Rockies

β-Ga_2O_3 has emerged as a leading candidate for next-generation power electronics, radio frequency (RF) switches, and extreme environment electronics due to a wide band gap (4.6 – 4.9 eV), high dopability (~40 meV activation energy for an isolated silicon donor), and melt growth characteristics resulting in commercially available 4-inch substrates and commercial demonstrations of 6-inch substrates by multiple techniques.

The (100) surface of Ga_2O_3 is highly desirable from a device and epitaxy standpoint – bulk growth of (100) material is more scalable than (010), the surface is nearly lattice-matched to p-type partner NiO, and Al_2O_3 incorporates at higher concentrations without phase separation. However, the epitaxial growth rate on (100) surfaces is less than 10% of other faces due to weak bonding and favorable desorption. Recent demonstrations have shown growth rate improvements from 0.4 nm/min to 1.5 nm/min by growing on (100) wafers that are offcut 6° in the -c direction.[1] These films show step-flow growth from (-201) step-edges and high electron mobility. Despite these exciting results, offcuts greater than 6° have not been explored due to the waste associated with grinding and polishing large offcuts.

In this talk we will discuss the molecular beam epitaxy (MBE) growth and properties of β-Ga_2O_3 grown on (100) substrates offcut in the -c direction up to 13.4°. These large offcuts are enabled by edge-fed film-defined growth (EFG) where the offcut is grown into the surface by pulling the crystal through the EFG die with the seed crystal rotated by the desired offcut angle. We will demonstrate that 13.4° offcut substrates still exhibit a terraced (100) surface, and that a >10x increase (4.8 nm/min) in growth rate is achieved. As previously reported on lower offcuts, we observe 100% reversal of substrate twin domains around the (001) direction at the substrate-epilayer interface. We will discuss electrical properties including record-low (by MBE) unintentional doping densities of < 5E15 cm^{-3}.

5:25pm **PCSI-MoA2-42 Direct Link between Duv-Induced amorphous SiO2 Compaction and Lens Aberration Drift - From Atomic-Scale Modeling to Field Optical Validation in Photolithography**, ***Kwang Hoon Lee**, Won Bo Lee,* Seoul National University, Republic of Korea

This study presents a comprehensive characterization of the dynamic interplay between atomistic interface evolution in amorphous SiO_2 projection optics and device-scale optical performance drift under deep ultraviolet (DUV, 193nm) exposure. By integrating large-scale molecular dynamics (MD) simulations with machine learning force fields and density functional theory (DFT) calculations, we unveil how DUV-induced local compaction and defect evolution at interfacial regions modulate both refractive index (n) and wavefront aberrations in operational lithography systems. Specifically, our results demonstrate a quantitative correlation between MD-tracked Si-Si bond fraction/density metrics and DFT-calculated optical constants, establishing a structure-property relationship essential for device-level transport and optical characterization.

Fleet-scale, in-field monitoring of photolithography scanners confirms that progression of Y-direction Zernike coma (WFE, Coma-Y) is aligned with simulation-predicted compaction-driven refractive index shifts, cementing the impact of interface-level atomic changes on macroscopic optical device performance. Notably, the transition from elastic to plastic compaction regimes leads to nonlinear escalation in WFE drift slopes, providing actionable thresholds for predictive maintenance and device calibration.

This work bridges atomistic simulation and high-volume manufacturing field data to deliver direct, actionable insights for the characterization and management of light transport, wavefront propagation, and functional reliability in advanced optical devices.

5:30pm **PCSI-MoA2-43 Strong Fermi-level Pinning Driven by Epitaxial Graphene Interlayer in Metal/4H-SiC Junction**, ***Eunseok Hyun**, Jungjae Park,* Ulsan National Institute of Science and Technology, Republic of Korea*; Junhyung Kim,* Electronics and Telecommunications Research Institute, Republic of Korea*; Jaehyeong Jo, Jiwan Kim, Hyunjae Park, Kibog Park,* Ulsan National Institute of Science and Technology, Republic of Korea

Fermi-level pinning is a phenomenon that the Schottky barrier of metal/semiconductor junction exhibits weak dependence on the metal work-function. According to the previous study [1], the metal/graphene/Si junction exhibits strong Fermi-level pinning which is expected on an ideal metal/Si junction. It has been reported that the Fermi-level pinning of metal/SiC junction is relatively weak compared with the metal/Si junction due to the ionicity between atomic elements of crystalline structure [2]. With this background, we investigated the Fermi-level pinning in metal/graphene/4H-SiC junctions. The junction was fabricated by first epitaxially growing graphene on a 4H-SiC substrate with the metal-capping method under UHV environment [3] and then depositing circular metal (Al, Ni, Pt) electrodes onto the grown graphene layer. The Fermi-level pinning factor S was extracted from current-voltage (I-V) and capacitance-voltage (C-V) curves, signifying strong Fermi-level pinning. A theoretical model proposed by Kopylov *et al*. describing the charge transfer at the graphene/SiC interface provides a plausible explanation for the observed strong Fermi-level pinning [4].

[1]Hoon Hahn Yoon *et al*., Nano Letters **17(1)**, 44 (2017)
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[3] Han Byul Jin *et al*.,Scientific Reports **5**, 9615 (2015)
[4] Sergey Kopylov *et al*., Applied Physics Letters **97**, 112109 (2010)

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5:35pm **PCSI-MoA2-44 UPGRADED: (Al)GaN/High-K Oxide Interface Formation: Insight from Time-Resolved Synchrotron Studies**, *Shreemoyee Chakraborty, Nishant Patel, Eleni Charitoudi, Erik Lind, Vanya Darakchieva,* ***Rainer Timm**,* Lund University, Sweden

The (ultra)wide bandgap semiconductors gallium nitride (GaN) and aluminum gallium nitride (AlGaN) are the materials of choice for enabling power electronic devices with very high switching frequency and superior energy efficiency. Such devices are based on metal-oxide-semiconductor (MOS) gate stacks, where downscaling and leakage control require gate oxides with high dielectric constant, so-called high-k oxides, such as HfO_2 [1]. However, device performance and especially switching frequencies are often limited by the insufficient quality of the (Al)GaN/high-k interface. Ultrathin, conformal high-k layers can be synthesized using atomic layer deposition (ALD), where the choice of oxide material, pre-ALD cleaning methods, and ALD parameters strongly influence film and interface quality. Many important details about the physics and chemistry of the interface formation still remain unknown. Furthermore, until now all efforts to explore the high-k oxide film formation have been based on ex situ approaches, meaning that film deposition and characterization of the resulting interface occur in separate steps.

Here, we present a first time-resolved investigation of the ALD reactions of HfO_2 on (Al)GaN. For this, we implemented the ALD process in a synchrotron ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) setup [2]. Thus, we mapped surface chemistry and electronic properties *in situ* during subsequent ALD half-cycles, which consisted of tetrakisdimethylamido-hafnium (TDMA-Hf) and water deposition. We observed a rather inefficient first ALD cycle, compared to previous semiconductor ALD studies [2], which improved with increasing aluminum content. Thickness and chemical composition of the resulting Hf-oxide film varied strongly if the order of the precursors was changed. Both observations are against the established ligand-exchange ALD model and highlight the importance of in-depth studies for improving the quality of high-k layers on (Al)GaN.

In addition, we have used XPS to systematically investigate the electronic properties and chemical composition of the interface between different (Al)GaN substrates and HfO_2 or Al_2O_3 high-k oxide films, for different ALD temperatures, where HfO_2 resulted in less interfacial oxide. The choice of pre-ALD cleaning methods (HCl or HF etching) was also found to be of importance, which can enhance ALD efficiency but also result in interface contamination. We will discuss how our structural results can be implemented to improve device performance.

[1] P. Gribisch et al., IEEE Trans. Electron Dev. 70, 4101 (2023).
[2] G. D'Acunto et al., ACS Appl. El. Mat. 2, 3915 (2020).

5:55pm **PCSI-MoA2-48 Structure and Transport Relationships of ZrN on MgO (001)**, ***Evangeline Beeching**,* Idaho National Laboratory

Combining superconducting metals with semiconductors provides the basis for many solid state devices including Josephson junctions, single electron transistors, and some photon emitters [1]. The interface between the superconductor and semiconductor can be a major source of loss in these devices, and the transport properties are highly intertwined with structural disorder and defects at various length scales. This project focuses on elucidating the role of disorder on superconductivity using thin films fabricated by molecular beam epitaxy, a deposition technique which

leverages precise control of stoichiometry, temperature, and substrate preparation. Using molecular beam epitaxy, we employ a method for controlling resulting disorder at the crystalline, structural scale and atomic scale resolutions.

ZrN thin films, a known superconductor, were deposited on various substrates and orientations across a range of growth conditions. Structural disorder is characterized using high-resolution x-ray diffraction. Additionally, 4-point contact schemes are used to analyze the effects of the structural disorder and determine the relationships with electrical transport down to cryogenic temperatures and under magnetic fields. These measurements reveal that the critical temperature of films deposited on MgO are below bulk critical temperature of 10 K, and some show steps indicative of multiple superconducting phases. The transport properties of ZrN on MgO are intimately related to the structural properties, which are found to depend on the nitrogen plasma conditions moreso than variations in substrate temperature. This somewhat contrasts observations on substrates with better lattice matching, which show quite a high dependence on substrate temperature. Disorder at a structural scale and atomic scale both arise, and can be somewhat independently controlled through tailoring the growth parameters. The understanding of disorder in epitaxial semiconductor-superconductor systems will pave the way for thin film based quantum devices.

PCSI

Room Ballroom South - Session PCSI-MoE

Oxides I

Moderator: Alex Demkov, The University of Texas

7:30pm **PCSI-MoE-1 Phonon Decoupling as a Route to Unit-Cell-Scale Ferroelectricity***, Yeongrok Jin,* ***Jaekwang Lee****,* Pusan National University, Republic of Korea **INVITED**

The ultimate scaling limit in ferroelectric switching has been attracting broad attention in the fields of materials science and nanoelectronics. Despite immense efforts to scale down ferroelectric features, however, only few materials have been shown to exhibit ferroelectricity at the unit-cell level.

Here we report a controllable unit-cell-scale domain in brownmillerite oxides [1] consisting of alternating octahedral/tetrahedral layers. Our machine-learning force-field (MLFF) phonon calculations reveal that the phonon modes related to oxygen octahedra are decoupled from those of the oxygen tetrahedra in brownmillerite oxides, and such localized oxygen tetrahedral phonons stabilize the sub-unit-cell-segmented ferroelectric domain (Fig.1) [2]. The discovery of unit-cell-scale ferroelectricity opens new possibilities for designing ultrahigh-density memory devices through phonon-mode engineering and interlayer decoupling [3].

[1] Y. Xing*, I. Kim*, K. T. Kang* *et al*., Nature Chemistry 17, 66-73 (2025).

[2] J. Jang*, Y. Jin*, Y. Nam* *et al*., Nature Materials 24, 1228 (2025).

[3] J. Hwang*, S. Jeong* *et al*., under review in Physical Review Letters (2025).

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8:10pm **PCSI-MoE-9 Accelerated Dielectric and Ferroelectric Materials Discovery by High-Throughput Thin Film Synthesis***, Aiping Chen,* LANL

Dielectric and ferroelectric materials are fundamental to modern electronic and energy storage technologies, enabling applications ranging from high-κ gate dielectrics to capacitors and nonvolatile memories. However, the discovery and optimization of new materials through conventional trial-and-error approaches remain slow and resource-intensive. Establishing a general-purpose platform that integratesmaterials informatics, combinatorial synthesis, and high-throughput characterization can dramatically accelerate the exploration of complex composition-structure-property relationships. Such an approach enables rapid mapping of materials phase space, identification of promising candidates, and iterative feedback between data-driven prediction and experimental realization, ultimately transforming the pace of dielectric and ferroelectric materials innovation.

In this talk, I will discuss our progress on developing high-throughput thin film synthesis for ferroelectric and dielectric thin films. In the first part, I will discuss the design of $(Ba_{0.7}Ca_{0.3})TiO_3$ (BCT) and $Ba(Ti_{0.8}Zr_{0.2})O_3$ (BZT) superlattices via a high-throughput combinatorial approach. In the second part of the talk, I will discuss strategies to further optimize domain structures and suppress the leakage current in BZT-BCT films via a machine learning approach. The large polarization and the delayed polarization saturation led to greatly enhanced energy density of 80 J/cm^3 and transfer efficiency of 85% over a wide temperature range. Such a data-driven design recipe for a slush-like polar state is generally applicable to quickly optimize functionalities of ferroelectric materials. Figure 1 shows the schematics of the combinatorial synthesis approach of growing the BCT-BZT thin films.

8:15pm **PCSI-MoE-10 Fabrication and Characterization of GeO_2/Ge-based MOS Capacitors after Controlled Adsorption of Water Molecules***, Hiroki Takano, Shuto Sano, Kouji Inagaki, Kenta Arima,* The University of Osaka, Japan

The GeO_2/Ge interface is known to generate positive fixed charges upon air exposure, posing challenges for device applications. Our research group has focused on the role of water molecules and their interaction with GeO_2/Ge surfaces. Using *in situ* X-ray photoelectron spectroscopy (XPS) with synchrotron radiated light, we systematically studied the relationship between relative humidity and the thickness of the adsorbed water layer. We also revealed substantial positive charging of GeO_2 films at humidity levels above 10^{-4}%, coinciding with the onset of water adsorption. While this effect was attributed to water penetration into the oxide, possible contributions from X-ray interactions complicated the interpretation.

In this talk, we present an investigation of the charging characteristics of GeO_2/Ge structures pre-exposed to controlled humidity conditions, evaluated through capacitance–voltage (*C*–*V*) measurements of metal-oxide-semiconductor (MOS) capacitors. To enable these experiments, we developed an integrated reaction chamber capable of annealing, controlled water adsorption, electrode formation via vacuum deposition, and electrical measurements on thermally oxidized GeO_2/Ge samples (550 °C) under high vacuum [1]. As part of the performance assessment of this system, MOS structures were fabricated on GeO_2/Ge structures exposed for 3 h to five different humidity levels (10^{-6}%, 0.01%, 0.1%, 0.9%, and 2.0 %) in the reaction chamber, as well as on an as-oxidized reference sample transported in air. The *C*–*V* curves of samples exposed to 1% RH or higher, as well as that of the as-oxidized sample, showed hysteresis and a significant negative shift. Furthermore, this hysteresis was identified as injection-type behavior. This phenomenon is attributed to the adsorption of water molecules onto the GeO_2/Ge structure at humidity higher than approximately 1% [1].

[1] S. Sano, H. Takano et al., J. Appl. Phys. **137**, 155304 (2025).

8:20pm **PCSI-MoE-11 Optical and Structural Characterization of Group-IV Oxides Produced by Rapid Thermal Annealing***, Haley Woolf, Danissa Ortega, Carlos Armenta,* New Mexico State University*; Matthew Mircovich, John Kouvetakis, Jose Menendez,* Arizona State University*;* ***Stefan Zollner****,* New Mexico State University

This project investigates the rapid thermal oxidation of Ge(Sn) on Si by examining their optical and structural changes. Group-IV oxides, particularly GeO_2, are promising piezoelectric materials suitable at high-temperature environments. As-received samples, prepared by chemical vapor depositino, underwent ultrasonic cleaning before oxidation. The samples were rapidly thermally oxidized at a pressure of 2.7 atm with an oxygen flow rate of 0.2 L/min. Spectroscopic ellipsometry measurements revealed that oxide thickness increased with both annealing temperature and time. Depolarizationand surface discoloration indicated non-uniformity within the oxide, which was incorporated into their optical modeling. X-ray diffraction confirmed formation of α-GeO_2. Reciprocal space maps were used to determine the strain state of the Ge epilayer and the relaxation/Sn content for the GeSn epilayer. The Deal-Grove model described Ge oxidation on Si, resulting in an activation energy of 4±2 eV for oxygen diffusion in Ge. The oxidation consumption rates for Ge and GeSn epilayers were determined to be 0.56-0.57 and 0.54, respectively.

8:25pm **PCSI-MoE-12 Surface Characterization of Implanted Arsenic on Si(100) Using Scanning Tunneling Microscopy and Spectroscopy***, Abigail Berg, Evan Anderson, DeAnna Campbell, Shashank Misra,* Sandia National Lab

Many quantum and classical device technologies require understanding tunneling in semiconductors, which are sensitive to defects in the tunnel barrier. Characterizing these defects is challenging because the devices involve heterogeneous interfaces and tight sub-10 nm dimensions. Meanwhile, it has been difficult to interpret data about the role of specific defects in semiconductors from scanned probe because of both the non-perturbative role of the tip and features of the electronic structure that are specific to surfaces [1][2][3][4]. Here, we present a method of identifying surface and subsurface features by creating local density of states (LDOS) maps using a scanning tunneling microscope at the surface of hydrogen-terminated silicon. We find that most defects that show up in the topography either do not show up in the LDOS maps or come from imperfections in the hydrogen passivation. By contrast, donors and acceptors are generally not visible in the topography, but can be detected as bright regions from the shift they impart in one of the band edges. The figure on the left provides an example of how we have identified different defects based on their LDOS. The grey boxes show dangling bonds which produce a high LDOS centered around zero bias, independent of the parent electronic structure. The blue and yellow boxes outline where there are donor and acceptor defects that produce bright features at the conduction and valence band edges in the LDOS. We also find some unexpected mid-gap defects in white. With this methodology in place, we plan on investigating mechanisms of dopant diffusion and defect formation more generally in devices ranging from tunnel field effect transistors to single-donor qubits.

8:30pm **PCSI-MoE-13 In_2O_3 Thin Films Deposited Using $InCl_3$ by Mist CVD Method***, Ryo Ishikawa, Tomohiro Yamaguchi, Takeyoshi Onuma, Tohru Honda,* Kogakuin University, Japan

In_2O_3 is an oxide semiconductor with high transparency and conductivity, widely used in transparent conducting films and channel layers of thin-film transistors (TFTs). For application to high-mobility TFTs, we have been studying the deposition of ~10 nm In_2O_3 films on SiO_2/Si substrates by the mist chemical vapor deposition (Mist CVD) method. Mist CVD is a technique

in which the precursor solution is atomized by ultrasonic vibration and thermally decomposed on a heated substrate. The precursor solution is typically prepared by dissolving metal powders in an acidic solvent such as HCl. In our previous studies, it was confirmed that decreasing the HCl concentration in the solution during Mist CVD resulted in thinner In_2O_3 films [1]. On the other hand, when the concentration approaches the solubility limit, undissolved In_2O_3 powder remains, which negatively affects the film quality. To address this issue, we focused on $InCl_3$ as an alternative precursor. Since $InCl_3$ is easily soluble in deionized water, HCl is not required to prepare the solution, and it is expected that thinner In_2O_3 films can be obtained simply by reducing the $InCl_3$ concentration [2]. In this study, In_2O_3 thin films were deposited on SiO_2/Si substrates by Mist CVD using $InCl_3$ solutions with concentrations between 0.0050 and 0.20 mol/L. The solutions were used after visually confirming complete dissolution by visual inspection.

Figure 1 shows the film thickness as a function of $InCl_3$ concentration measured using SE and TEM. The results show that the In_2O_3 films became thinner as the $InCl_3$ concentration decreased.An In_2O_3 film thickness of about 10 nm was achieved at the concentration of 0.0050 mol/L. Figure 2 shows the bird's-eye FE-SEM images of In_2O_3 films grown at the $InCl_3$ concentrations of 0.0050 and 0.20 mol/L. At the concentration of 0.0050 mol/L, the smoother surface was obtained with smaller crystal grain sizes, while at 0.20 mol/L, the three-dimensional surface was obtained with large crystal grain sizes. The flattening of the surface with decreasing $InCl_3$ concentration can be explained by the smaller grain size. In the presentation, we will comprehensively discuss the structure of the grown In_2O_3 thin films, including their electrical properties.

8:35pm **PCSI-MoE-14 UPGRADED: Quantum Interference at the $(La_{0.3}Sr_{0.7})(Al_{0.65}Ta_{0.35})O_3/SrTiO_3$ Interface***, **Km Rubi**,* Los Alamos National Laboratory*; Kun Han, Huang Zhen,* National University of Singapore*; Michel Goiran, Duncan Maude, Walter Escoffier,* Laboratoire National des Champs Magnétiques Intenses, Toulouse, France*; Ariando Ariando,* National University of Singapore

Quantum interference – whether observed in the form of Aharonov-Bohm effect, the Altshuler–Aronov–Spivak effect, or quantum conductance fluctuations – offers valuable insights into electron dynamics within an electromagnetic environment. These phenomena allow direct measurement of the phase coherence length, which is critically important for developing quantum technologies such as quantum sensing, quantum computing, and quantum communication.

We report quantum oscillations in magnetoresistance that are periodic in magnetic field (B), observed at the interface between $(La_{0.3}Sr_{0.7})(Al_{0.65}Ta_{0.35})O_3$ and $SrTiO_3$ [1]. Unlike Shubnikov–de Haas oscillations, which appear at magnetic fields > 7 T and diminish quickly as the temperature rises, these B-periodic oscillations emerge at low fields and persist up to 10 K. Their amplitude decays exponentially with both temperature and field, specifying the dephasing of quantum interference. Increasing the carrier density through electrostatic gating results in a systematic reduction in both the amplitude and frequency of the oscillations, with complete suppression beyond a certain gate voltage. We attribute these oscillations to the Altshuler–Aronov–Spivak effect, likely arising from naturally formed closed-loop paths due to the interconnected quasi-one-dimensional conduction channels along $SrTiO_3$ domain walls. The relatively long phase coherence length (~ 1.8 μm at 0.1 K), estimated from the oscillation amplitude, highlights the potential of complex oxide interfaces as a promising platform for exploring quantum interference effects and advancing device concepts in quantum technologies, such as mesoscopic interferometers and quantum sensors.

PCSI
Room Ballroom South - Session PCSI-TuM1
Oxides II

Moderator: Jaekwang Lee, Pusan National University

8:30am **PCSI-TuM1-1 What Are High Entropy Ceramics and What Are They Good for?**, ***Alessandro Mazza,*** Los Alamos National Laboratory **INVITED**

Disorder has long been a tool in changing mechanical, electronic, and other physical properties of materials. However, the amount of control is regularly limited by the enthalpy of formation for high concentrations of dopants/adatoms. As a mechanism to overcome this limitation, high entropy ceramics increase the number of elements on lattice sites – thereby lowering the overall Gibbs free energy of formation by increasing the configurational entropy of the system. Using this method, theoretical and experimental results exploring the role of disorder at this scale in manipulating spin, charge, lattice and electronic order parameters will be discussed. First, in exploring magnetism, electronic structure and valence of the high entropy ABO_3 perovskite $La_{1-x}Sr_x(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$. Second, in an experimental realization of extreme *A*-site cation disorder in $(Y_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}Gd_{0.2})NiO_3$, whose parent ternary oxides each have a large range of electronic (metal to insulator transition) and structural phase transition temperatures. In exploring these systems, it is revealed that disorder on this scale can suppress or favor certain order types, create phase frustration, and be used to design a desired phenomena not accessible by conventional materials design methods.

9:10am **PCSI-TuM1-9 Atomic Layer Deposition of Cr_2O_3: Comparing Ozone and Plasma Routes for TFTs**, ***Soumik Das,*** *Arka Sardar,* imec USA; *Sean McMitchell,* IMEC Belgium; *Becky (R. L.) Peterson,* University of Michigan, Ann Arbor

Chromium(III) oxide (Cr_2O_3) is a wide-bandgap p-type semiconductor of interest for thin-film transistors (TFTs) and spintronic devices, where complementary p-type oxides are needed to pair with high-performance n-type materials such as ZnO and IGZO. Atomic layer deposition (ALD) provides the precision and conformality essential for device integration. In this work, we investigate Cr_2O_3 growth from $Cr(acac)_3$ using ozone and oxygen plasma as oxidants. Plasma introduces highly reactive species that remove ligands efficiently at lower temperatures, while ozone promotes combustion-like oxidation that can enhance growth but also drive etching depending on exposure. Initial results show plasma ALD achieves sub-0.1 Å/cycle growth, though etching competes with deposition, whereas ozone requires higher substrate temperatures but produces crystalline films. Current efforts focus on optimizing precursor dosing and temperature windows to control stoichiometry and reduce defect density. Looking forward, we will fabricate and benchmark TFTs from both ozone and plasma-grown films to directly compare performance. This work will clarify how oxidant choice shapes Cr_2O_3 film quality and device behavior, guiding its use as a p-type channel in future oxide electronics and spintronics.

9:15am **PCSI-TuM1-10 Correlated Oxygen States and Schottky Barrier Height in Transition Metal Oxides from First Principles**, ***Sohm Apte,*** *Alexander Demkov,* University of Texas at Austin

Schottky barrier height (SBH) [1] that measures the potential barrier for charge transfer across a metal-semiconductor interface, is one of the central quantities for semiconductor and electro-optic devices. SBH directly affects contact resistance, rectification, leakage current, and turn-on voltage. As such, accurately predicting Schottky barrier heights from first principles is of crucial scientific and technological importance.

In the ideal Schottky-Mott picture [2], the SBH is simply defined as the difference between the work function of the metal and the electron affinity of the semiconductor. However, in real materials the presence of interface dipoles, chemical bonding, metal-induced gap states and defect-driven Fermi-level pinning, makes the determination of the SBH extremely complicated. In particular semi-local density functional theory (DFT) suffers from a self-interaction error which results in underestimated band gaps and misaligned band edges [3]. In transition-metal oxides, a common remedy is to add a Hubbard U term on the transition metal d-orbitals that form the conduction band bottom [4]. While this strategy improves bulk gaps and d-state localization, it often remains insufficient for interfaces. For several materials the calculated barrier heights significantly deviate from experimental values unless much more expensive methods like GW are employed.

Many transition metal oxides have tops of their valance bands comprise oxygen 2p states with a relatively flat dispersion. These bands have a large effective mass and are particularly susceptible to self-interaction error, leading to a distortion in the band alignment at the interface. This observation motivates treating the oxygen 2p electrons as correlated degrees of freedom. In this work we show that introducing a Hubbard U on the oxygen 2p states systematically lowers the valence manifold, corrects the offsets, and yields quantitatively accurate barrier heights. We demonstrate this idea by choosing ten candidate oxides and constructing an interface with platinum. Platinum is a high work-function, chemically stable contact that is widely used experimentally. Importantly platinum does not readily scavenge oxygen under typical growth conditions. Beyond improving agreement, our approach is computationally efficient relative to hybrid functionals or many-body perturbation theory, making it practical for material screening and device-scale modeling.

[1] W. Schottky, Z. Phys. 113, 367 (1939)

[2] N. F. Mott, Proc. R. Soc. (London) A 171, 27 (1939)

[3] J. P. Perdew, International Journal of Quantum Chemistry 28, 497 (1985)

[4] R. T. Tung, Applied Physics Reviews 1, 011304 (2014)

9:25am **PCSI-TuM1-12 Coherent X-Ray Studies of Spontaneous Fluctuations in Rare Earth Nickelates**, ***Roopali Kukreja,*** University of California at Davis **INVITED**

Rare-earth nickelates ($RNiO_3$) exhibit a rich interplay of electronic, magnetic, and structural phase transitions, including a metal-to-insulator transition (MIT) [1]. While these transitions have been widely studied, spontaneous fluctuations across the phase transition are mostly unexplored. Such fluctuations are increasingly recognized for enabling stochastic functionality in neuromorphic computing. Here, we employ X-ray photon correlation spectroscopy (XPCS) [2-3] to directly probe structural and magnetic fluctuations in $NdNiO_3$ and $SmNiO_3$ thin films. For $NdNiO_3$, we observe a pronounced slowdown in fluctuation timescales—by an order of magnitude—near the Néel temperature, highlighting strong coupling between structural and magnetic order parameters, independent of epitaxial strain. In contrast, $SmNiO_3$ shows no such slowdown. Unexpectedly, wavevector-dependent measurements reveal that short-range structural fluctuations are significantly slower (by a factor of 3–5) than long-range fluctuations [4]. Our results demonstrate the power of coherent X-ray techniques in capturing nanoscale fluctuation dynamics and provide new insight into the role of fluctuations in complex oxides.

1. Middey S., Chakhalian J., Mahadevan P., Freeland J. W., Millis A. J., Sarma D. D. Physics of ultrathin films and heterostructures of rare earth nickelates. Annual Review of Materials Research 46, 305 (2016)
2. Sinha S. K., Jiang Z., Lurio L.B. X-ray photon correlation spectroscopy studies of surfaces and thin films. Advanced Materials 26, 7764 (2014)
3. Shpyrko O.G. X-ray photon correlation spectroscopy. Journal of Synchrotron Radiation 21, 1057 (2014)
4. Zhou Hagstroem, N. et al. Critical slowdown of spontaneous fluctuaitons in the vicinity of metal-insulator transition in rare earth nickelates, in review (2025).

PCSI
Room Ballroom South - Session PCSI-TuM2
Atomic Layer Deposition

Moderator: Jessica Hilton, SPECS-TII, Inc.

11:00am **PCSI-TuM2-31 X-ray Photoemission Spectroscopy for Non-Destructive Analysis of Si Trench Bottoms**, ***Shiika Murase,*** *Tomoki Higashi, Taizo Kawashima, Kouji Inagaki, Kenta Arima,* The University of Osaka, Japan

Three-dimensional (3D) structures with high aspect ratios (ARs) have become standard in highly integrated semiconductor devices [1,2]. Ensuring high yield requires stringent cleanliness; however, non-destructive evaluation of cleaning in 3D structures remains limited, despite extensive studies on flat surfaces. To address this issue,we aim to develop a novel non-destructive method for evaluating cleaning performance at the bottoms of 3D nanostructures. Specifically, we apply angle-resolved X-ray photoemission spectroscopy (AR-XPS) to 3D structures such as deep trenches, embedding heterogeneous “landmark” elements selectively embedded at the bottoms as vertical markers.

In this talk, we examine the feasibility of the proposed method by obtaining XPS spectra of Si trenches with different ARs (1–7). To this end, Si trench

structures were fabricated with gold (Au) selectively embedded at the bottoms using a wet etching process known as metal-assisted chemical etching (MACE) [3, 4]. AR-XPS measurements of these structures revealed a strong take-off angle (TOA) dependence of the Au 4f signal, particularly at higher ARs. This indicates that the embedded Au serves as an effective marker for aligning the sample and detector axes. AR-XPS was also conducted after removing Au from the trench bottoms.The resulting Si 2p spectrum exhibits a clear component corresponding to bulk Si(Fig. 1b), clearly distinguishable from that of Au-embedded samples (Fig. 1a), indicating that the signal originates from the trench bottoms. In other words, Fig. 1 demonstrates that MACE-fabricated Si trenches possess chemically distinct surface conditions at the top and bottom, enabling separation in Si2p XPS spectra without additional surface treatments [5].The proposed method is expected to be used in evaluating wet and dry cleaning processes at the bottoms of high-aspect-ratio structures.

11:05am **PCSI-TuM2-32 Interface Energy Barrier Inhomogeneity of Pt/4H-SiC Junction Probed with Planar Ballistic Electron Emission Spectroscopy**, ***Jiwan Kim***, *Jaehyeong Jo, Jungjae Park, Hyunjae Park, Eunseok Hyun, Jisang Lee, Sejin Oh, Kibog Park,* Ulsan National Institute of Science and Technology, Republic of Korea

The inhomogeneity of the interfacial energy barrier is associated with crystallographic variations of the interface, which is inevitable in heterojunctions. The ballistic electron emission microscopy/spectroscopy (BEEM/BEES) has been commonly used to observe the local variation of interfacial energy barrier with high spatial resolution (1-10 nm) [1]. However, the tip-related issues [2, 3] and long scanning time make it difficult to investigate the large area reliably. Here, we suggest an experimental methodology utilizing the device version of BEES to estimate the inhomogeneity of interfacial energy barrier with single spectral measurements covering the entire junction area. Our approach (*i*) relies on the Bell-Kaiser theory [1] for a 'point' BEEM response, (*ii*) treats the tunnel junction as an ensemble of virtual BEEM tips, and (*iii*) models the second-derivative spectrum (SDS) of the 'lumped' BEEM response using a known statistical nature of interfacial barriers [4]. For the case of simple two distinct Schottky barriers (SBs), the working principle of 'planar BEES' is illustrated in Fig. 1. To validate our methodology, we apply it to Pt/4H-SiC junction, adopting the Gaussian distribution of interfacial barriers. In its SDS (see Fig. 2), we observe two peaks at 1.60 V and 1.74 V corresponding to two lowest conduction band minima of 4H-SiC located at the M point of the Brillouin zone [5] and the standard deviation of SB is obtained to be 156.7 meV. Our methodology can be used broadly for other heterojunctions as long as the inhomogeneous interface possesses the Gaussian nature.

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11:10am **PCSI-TuM2-33 Porous W2N Fibrous-Nanograins and TiN Nanopyramids Framework for High Energy Density Flexible Asymmetric Supercapacitors**, ***Rajesh Kumar***, *Bhanu Ranjan, Davinder Kaur,* Indian Institute of Technology Roorkee, India

Enhancing the energy density of flexible asymmetric supercapacitors (ASCs) necessitates developing and implementing high-performance anode materials for technological developments in wearable energy storage systems. Tungsten nitride (W_2N) offers enormous potential as an anode material for ASCs, ascribed to its substantial specific capacitance, massive electrical conductivity, and extended negative potential window. In this work, we fabricated a durable coin cell and flexible ASC utilizing W_2N/SSM fibrous-nanograins anode and TiN/SSM nanopyramids cathode deposited over flexible stainless steel mesh (SSM) substrate by the DC magnetron sputtering technique. The W_2N/SSM//TiN/SSM ASC device demonstrates a high areal capacitance of 21.3 $mF.cm^{-2}$ operating across a wide and stable electrochemical voltage window of 1.3 V with outstanding cycling robustness demonstrating 89.09% retention over 8000 charge-discharge cycles. Notably, the ASC achieved a high energy density of 34.33 $mWh.cm^{-3}$ and a high power density of 17.32 $W.cm^{-3}$. The persistent electrochemical performance of ASC is mainly attributed to the dominance of surface-controlled capacitive and pseudocapacitive charge storage kinetics of W_2N/SSM for Na^+ ions comprehensively examined employing 3D Bode and Dunn's techniques. The flexible ASC shows remarkable mechanical stability of 92.36% up to 500 bending cycles. This study establishes W_2N nanograin's potential as a high-energy anode material, revealing the capability to increase the effectiveness of ASC for portable and miniaturized energy storage devices.

11:15am **PCSI-TuM2-34 Magnetocrystalline Anisotropy as a Design Principle in PtPdFe Intermetallic Alloys for Fuel Cell Electrocatalysis**, *Muhammad Irfansyah Maulana, DongHyun Lee,* ***Jong-Sung Yu***, DGIST, Republic of Korea

Ordered Pt-based intermetallic alloys are emerging as efficient oxygen reduction reaction (ORR) electrocatalysts in hydrogen fuel cells, outperforming their disordered counterparts. However, the intrinsic role of atomic ordering in governing ORR catalytic performance remains unclear. In this work, we report ferromagnetic PtPdFe ternary intermetallics with structurally ordered tetragonal $L1_0$ and cubic $L1_2$ phases (Figure 1a), each featuring distinct crystal structures and atomic arrangements. Our study highlights magnetocrystalline anisotropy as a key structure-dependent descriptor that governs ORR activity in these alloys. Electrochemical half- and single-cell tests reveal that $L1_0$-PtPdFe magnetic intermetallic catalysts (MICs) deliver higher ORR activity than their $L1_2$ counterparts (Figure 1b). Combined experimental and theoretical analyses attribute this enhancement to the unique tetragonal $L1_0$ structure, where strong 5d–3d orbital interactions along the c-axis induce ferromagnetic ordering and elevate magnetocrystalline anisotropy energy, thereby accelerating ORR kinetics. Furthermore, membrane electrode assemblies fabricated by $L1_0$-PtPdFe cathode MICs sustain fuel cell performance beyond the 2025 US Department of Energy stability targets under H_2–O_2, H_2–air, and H_2–N_2 conditions. These findings establish a new design principle for Pt-based intermetallic catalysts, demonstrating that magnetic anisotropy arising from ferromagnetic ordering can be strategically harnessed to optimize fuel cell performance.

11:20am **PCSI-TuM2-35 Orientated Deposition of Li_2S for Fast-Charging Lithium-Sulfur Batteries**, ***Jeong-Hoon Yu***, *Donghyun Lee, Jong-Sung Yu,* DGIST, Republic of Korea

Precipitation/dissolution of insulating Li_2S has long been recognized as the rate-determining step in lithium–sulfur (Li–S) batteries, which dramatically undermines sulfur utilization at elevated charging rates. Herein, we present an orientated Li_2S deposition strategy to achieve extreme fast charging (XFC, ≤15 min) through synergistic control of porosity, electronic conductivity, and anchoring sites of electrode substrate [1]. Via magnesiothermic reduction of a zeolitic imidazolate framework, a nitrogen-doped and hierarchical porous carbon with highly graphitic phase was developed. This design effectively reduces interfacial resistance and ensures efficient sequestration of polysulfides during deposition, leading to (110)-preferred growth of Li_2S nanocrystalline between (002)-dominated graphitic layers. Our approach directs an alternative Li_2S deposition pathway to the commonly reported lateral growth and 3D thickening growth mode, ameliorating the electrode passivation. Therefore, a Li–S cell capable of charging/discharging at 5 C (12 min) while maintaining excellent cycling stability (82% capacity retention) for 1000 cycles is demonstrated. Even under high S loading (8.3 mg cm^{-2}) and low electrolyte/sulfur ratio (3.8 µL mg^{-1}), the sulfur cathode still delivers a high areal capacity of >7 mAh cm^{-2} for 80 cycles.

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11:25am **PCSI-TuM2-36 Platforms for Boundary-Controlled Synthesis of Screw Dislocations in Single-Crystalline Semiconductors**, ***Zachary Handoklow***, University of New Mexico

We present our efforts on the fabrication of materials platforms to investigate boundary-controlled synthesis of screw dislocations. Our developed structures are based on twisted bicrystals formed by single-crystalline nanomembranes of various thicknesses bonded onto a bulk crystal of the same chemical and physical structure.

11:30am **PCSI-TuM2-37 Substrate-Strain-Controlled Molecular Beam Epitaxial Growth and Scanning Tunneling Microscopy of Antiperovskite Mn_3GaN**, ***Ali Abbas***, Ohio University; *Juan Carlos Moreno Hernandez,* Universidad Autonoma de Puebla, Mexico; *Ashok Shrestha,* Ohio University; *Daniel Russell, Fengyuan Yang,* Ohio State University; *Kai Sun,* Michigan State University; *Arthur R. Smith,* Ohio University

This study investigates the epitaxial growth, structural characterization, and theoretical modeling of thin-film antiperovskite Mn_3GaN, a chiral antiferromagnetic material with a kagomespin lattice grown on MgO (001) substrates via nitrogen plasma-assisted molecular beam epitaxy (MBE). The

resulting films exhibit a homogeneous composition with atomically smooth surfaces and sharp interfaces, characterized by minimal in-plane tensile strain and out-of-plane compressive strain. First-principles calculations are employed to determine the energetically favorable configurations of both the MGN surface and the MGN /MgO heterostructure, and STM images reveal an atomically smooth surface with atomic-height steps [1].

The results show that the MnGa layer along the (001) direction is energetically favorable [1]. This layer is ferromagnetic in-plane, whereas in the (111) plane, all Mn3Ga layers have chiral antiferromagnetic spin structure, making these very interesting from the spin perspective. In principle, this spin structure is accessible via spin-polarized STM, which is currently our aim. Furthermore, measurements at low temperatures can be accomplished using our new variable-temperature STM system, which enables better tip stability and lower noise. Since the Neel temperature of Mn3GaN is 298 K, by investigating this system using spin-polarized STM tips at cryogenic temperatures, it is possible to resolve the temperature-dependent spin structure, and even the Neel transition.

This research has been supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317 (MBE, RHEED, STM) and under award No. DE-SC0001304 (XRD, SQUID).

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PCSI

Room Ballroom South - Session PCSI-TuE

Is AI a Bubble?

Moderator: Alping Chen, Los Alamos National Laboratory

7:00pm **PCSI-TuE-1 AI-Accelerated Discovery of Emergent Properties in 2D Materials and Moiré Superlattices**, ***Ting Cao***, University of Washington **INVITED**

Moiré superlattices formed in twisted and stacked 2D materials offer a powerful platform for engineering interfacial electronic and optical properties. Their vast supercells and complex reconstructions, however, challenge the limits of conventional first-principles methods. In this talk, I will present machine-learning assisted first-principles calculations that enable large-scale simulations of moiré structures, capable of handling twisted multilayer homo and heterostructures with varying composition, twist angles, stacking, and layer numbers.

Demonstrated on twisted MoTe2, our calculations capture topology-driven band transitions and provide a scalable solution for studying correlated moiré phenomena in complex environment, predicting emergent electronic features such as flatter Chern bands. The emergent moiré potentials and band structures in turn govern the behavior of excitons with unusually large dipole moments and tunable spatial profiles. By incorporating spin–lattice descriptors, the same machine-learning assisted framework reveals pathways to coupled excitonic and magnetic responses.

Our AI-accelerated strategy extends the predictive reach of first-principles theory, providing new insights into how twist angle, stacking order, and electric control can be used to design moiré materials with tailored optical, electronic, and spin functionalities**.**

7:40pm **PCSI-TuE-9 Full-Field Structural Microscopy Reveals Dynamic Film–Substrate Interactions in VO_2 Neuromorphic Devices**, ***Alex Frano***, University of California San Diego **INVITED**

Understanding how structural transitions govern neuromorphic functionality in quantum materials requires characterization tools that can probe local transformations in operando and across multiple length scales. We combine dark-field X-ray microscopy (DFXM) with complementary X-ray and electron microscopies to reveal the structural evolution of voltagedriven filaments in VO_2 memristive devices and their unexpected coupling to the underlying substrate. DFXM provides high-resolution, full-field, structure-selective imaging, enabling us to visualize rutile filament formation without destructive specimen preparation or slow rastering. We find [1] that rutile channels contain residual monoclinic clusters, revealing internal nonuniformity, and that rutile nucleation beneath electrodes precedes the Figure 1: A schematic of DFXM growth of conductive pathways. Additionally, imaging filamentary domains in a VO2 repeated voltage cycling induces a medium-term (<30 neuromorphic device. min) memory effect: specific sites in the device gap switch at lower voltages even after a brief thermal reset. Strikingly, we show [2] that these electronic/structural transformations in the VO_2 film are not mechanically isolated: filament formation generates strong, highly asymmetric strain fields that imprint deep into the Al_2O_3 substrate. This strain feeds back into the film, guiding subsequent filament expansion and redefining local switching dynamics. The observed film–substrate feedback mechanism expands the conventional view of epitaxial strain from a static constraint to an active, reconfigurable parameter during device operation. These results position DFXM as a powerful platform for operando studies of correlated oxides and point toward substrate engineering as an emerging route to control and functionalize neuromorphic architectures.

PCSI

Room Ballroom South - Session PCSI-WeM1

2D Materials

Moderator: Ursula Wurstbauer, University of Münster

8:30am **PCSI-WeM1-1 Flat Bands and Excitons in Transition Metal Dichalcogenide Moiré Patterns**, ***Mit Naik***, University of Texas at Austin **INVITED**

Moiré patterns of 2D van der Waals materials have proven to be an ideal platform to host unusual correlated electronic phases, emerging magnetism, and exciton physics. At small twist-angles, novel moiré exciton states in transition metal dichalcogenide (TMD) heterostructures have been recently discovered through the observation of multiple emergent peaks in the optical spectra, but their atomistic nature has been a mystery. Using first-principles GW-Bethe Salpeter equation calculations we discover a rich diversity of excitonic states in large-area TMD moiré superlattices, particularly a novel exciton with an intralayer charge-transfer character. We uncover a complex interplay between structural reconstruction, the formation of flat bands, and the nature of excitonic states. These studies, which involve thousands of atoms in the reconstructed moiré unit-cell, are made feasible by the development of a new computational approach

While small twist-angles have been widely studied, large twist angle superlattices are often considered electronically layer-decoupled due to misaligned Brillouin zones of the individual layers. Surprisingly, we observe the emergence of flat electronic bands with a distinctive anisotropic dispersion at a large magic twist angle in TMD bilayers. A direct consequence of this flat band is the emergence of phonon-assisted intervalley absorption peaks in reflection contrast spectra measurements. The flat band shows a power-law divergent density of states due to its quasi-one-dimensional character, enhancing the potential for correlated phases.

9:10am **PCSI-WeM1-9 Impact of External Screening on the Valence and Core-Level Photoelectron Spectra of One-Layer WS_2**, *Alex Boehm, Chris Smyth, Andrew Kim, Don Bethke, Tzu-Ming Lu,* Sandia National Laboratories*; Jose Fonseca Vega,* Naval research Laboratory*; Jeremy Robinson,* naval research Laboratory*;* ***Taisuke Ohta****,* Sandia National Laboratories

In an effectively-screened environment, transition metal dichalcogenides (TMDs) rearrange their charge carriers to screen the added charges, and reduce the electronic band gap. Consequently, when interfaced with dissimilar materials, a sheet of TMD would change its band gap adapted to its local external screening environment. Similarly, a well-screened environment stabilizes photo-holes or core-holes created in the photoemission process and, in turn, boosts the kinetic energy of photoelectrons resulting in the apparent smaller binding energy. Complication arises when determining the electronic band alignment of TMDs using photoelectron spectroscopy since the screening influences the material property of interest as well as its assessment approach concurrently. Using a sample that contains areas of suspended and gold-supported one-layer WS_2, we show how the electronic states of WS_2 under the contrasting effective or ineffective external screening environment align at the built-in junction. The photoelectron spectra point to the breakdown of rigid shifts between the valence states and core-levels with the core-levels shifting more than twice as much as the valence states. Additionally, effectively-screened WS_2 displays a valence state with a substantially larger photoemission linewidth than ineffectively-screened suspended WS_2. Altogether, our result provides key insights into how the local variation of the external screening environment creates essentially a heterojunction within a layer of WS_2, and whether commonly accepted photoelectron spectroscopy practices hold when examining the electronic structures of one-layer TMDs.

The work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories and Base Programs and the Nanoscience Institute at the Naval Research Laboratory via the Office of Naval Research. A.R.K. acknowledges support from the U.S. Department of Energy, Office of Science, Division of Materials Sciences and Engineering (grant BES 20-017574). Samples were fabricated, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the US Department of Energy, Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly-owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

9:15am **PCSI-WeM1-10 Disorder-Induced 2D to 3D Dielectric Screening Transition in Single-Layer WS2**, ***Christopher Smyth***, *Alex Boehm,* Sandia National Laboratories*; Kory Burns,* University of Virginia*; Catalin Spataru, Andrew Kim, Don Bethke, Tzu-Ming Lu, Taisuke Ohta,* Sandia National Laboratories

The quasiparticle band gap ($E_{g,QP}$.) and dielectric permittivity represent fundamental properties of bulk semiconductors as a result of the three-dimensional (3D) character of the dielectric screening. In two-dimensional (2D) materials, the lattice is confined well below the typical dielectric screening length, and the non-local characteristic of the dielectric function emerges, resulting in unusually large exciton radius and binding energy in the weak screening environment. Consequently, the $E_{g,QP}$ and exciton binding energy become highly responsive to perturbations in the dielectric screening with extrinsic origins. Ubiquitous monovacancies in 2D semiconductors host a polarizable dipole, which can impact the screening strength and $E_{g,QP}$ through the internal defect density (n_v). Similarly, substrate-induced screening can impact the $E_{g,QP}$ and exciton behavior, which often obscures the combined effects of multiple screening mechanisms.

We present an experimental investigation of the isolated and combined impacts of structural disorder and external dielectric screening on the $E_{g,QP}$ and exciton behavior in single-layer WS_2. Introducing dilute structural disorders, primarily sulfur monovacancies, to weakly screened WS_2 results in a significant 190 meV renormalization of the $E_{g,QP}$, while the optical bandgap remains effectively unchanged at around 2.0 eV, as confirmed by photoemission spectroscopy (PES) and electron energy loss spectroscopy (EELS). When the n_v reaches a threshold of 5×10^{12} cm^{-2}, the interactions between isolated excitons and defects in poorly screened WS_2 transition to correlated interactions. The exciton-defect interaction changes because the screening radius and interdefect distance converge at ~4 nm. The emergence of correlated exciton-defect interactions is attributed to the dielectric function transitioning from a 2D to 3D character. In contrast, the $E_{g,QP}$ and exciton binding energy of WS_2 remain unaffected by vacancies when the screening environment is dominated by a strongly screening Au substrate. Therefore, the sensitivity of the electronic band structure and exciton stability in 2D materials to the screening environment hinges on their polarizability.

This work was supported by a LDRD program at SNL. A.R.K. acknowledges support from the U.S. DOE SC, Division of MSE. SNL is a multimission laboratory managed and operated by NTESS, LLC, a subsidiary of Honeywell International, Inc., for the NNSA under contract DE-NA-0003525. The views expressed in the correspondence do not necessarily represent the views of the U.S. DOE or the U.S. Government. This work was performed, in part, at CINT, a User Facility operated for the U.S. DOE SC.

9:20am **PCSI-WeM1-11 Tuning Phonon and Exciton Dynamics Through Alloying in 2D Transition Metal Dichalcogenides**, ***Tinsae Alem***, *Hayden Barry, Stephen McDonnell,* University of Virginia*; Jordan Hachtel,* Oak Ridge National Laboratory*; Chris Smyth,* Sandia National Laboratories*; Kory Burns,* University of Virginia

Quasiparticles play a key role in thermal transport and electronic behavior in 2D materials, where dipole interactions and lattice dynamics can be tuned via compositional alloying. However, controlling momentum transitions of phonons, coupling strength of excitons, and their locality based on intrinsic stresses in the lattice remains a challenge. This is attributed to a limitation in bulk characterization techniques; they give global information that averages thousands of unit cells, making it impossible to correlate which bonds result in individual displacement modes or optical transitions. Hereby, we investigate how alloying in $W_xMo_{1-x}S_2$ modulates local dipole moments and phonon/exciton populations, with implications for thermoelectric performance. By varying stoichiometry across five compositions, we examine how vibrational properties evolve with atomic-scale disorder and dipole perturbation. Bulk vibrational modes were measured using Raman and Infrared (IR) spectroscopy, with Raman providing superior energy resolution and enabling the collection of low-energy optical phonons. The optical spectrum was interpreted with photoluminescence (PL) to measure band transitions and splitting in the valence band. To access vibrational and optical behavior beyond the diffraction limit set by the wavelength of photons, we used monochromated electron energy loss spectroscopy (EELS) inside an aberration-corrected scanning transmission electron microscope (STEM),

enabling atomic-scale mapping of phonon and exciton populations. X-ray photoelectron spectroscopy (XPS) and energy-dispersive X-ray spectroscopy (EDX) confirmed chemical uniformity over micron and nanometer length scales. This combined approach reveals how alloying influences spin-orbit coupling and lattice vibrations, offering insight into thermal transport and tunability of exciton-phonon coupling in low-dimensional semiconducting platforms.

9:25am **PCSI-WeM1-12 UPGRADED: Quantum Emitters from Electrostatically Strained WSe2 Monolayers Suspended Over Nanocavities**, ***Frances Camille Wu***, *Jadon Zheng, Shang-Hsuan Wu, Bin Fang, Edward Yu,* The University of Texas at Austin

Tungsten diselenide (WSe_2) monolayers are promising hosts for quantum emitters due to their intrinsic dark exciton state, which hybridizes with defect states under tensile strain, resulting in localized defect emission. To date, strain engineering has focused primarily on creating static strain via techniques such as draping WSe_2 monolayers on patterned substrates or indentation with an atomic force microscope, which suffers from poor control over strain. In this study, we employ an electrostatic straining approach demonstrated for monolayer WSe_2 suspended over micron-scale cavities in a patterned substrate. In this approach, a back-gate voltage applied to the silicon substrate below the cavity induces a downward deflection of the suspended WSe_2 monolayer due to the capacitive interaction between the monolayer and substrate.[1]

Here, we investigate scaling of the cavity to nanoscale dimensions, allowing the distance between emitters to be smaller than the wavelength of light and enabling the study of cooperative emission behaviors from coupled emitters such as those leading to superradiant emission. This collective emission from coupled emitters has been previously observed in laterally arranged quantum dot ensembles, but not in highly scalable WSe_2-based quantum emitters. By performing electrostatic straining on a WSe_2 monolayer suspended over 100-nm diameter cavities, monolayer deflections of 2 nm (V_g = 10 V) and 3.5 nm (V_g = 27.5 V) were observed, corresponding to 0.2 and 0.4% increase in tensile strain, respectively. Initial studies of photoluminescence from a WSe_2 monolayer suspended over 10 cavities showed a linear (rather than saturating) behavior of localized emitter intensity as a function of increasing excitation power, a distinct characteristic of cooperative emission. Second-order photon correlation measurements showed an emitter antibunching behavior of $g^{(2)}(0)$ = 0.24±0.03, indicative of high-purity emitters, which can be attributed to the effective exciton funneling on nanoscale cavities. Current studies are focused on the electrostatic biasing of the suspended WSe_2 monolayer, which could enable precise strain modulation and enhanced coupling of emitters for possible observation of additional cooperative emission phenomena. This can be beneficial for the development of highly scalable and tunable coupled quantum emitters from strained WSe_2 monolayers for potential applications in quantum information processing, quantum laser technology, and quantum computing.

PCSI
Room Ballroom South - Session PCSI-WeM2
Crystal Growth

Moderator: Christopher Palmstrøm, University of California, Santa Barbara

11:00am **PCSI-WeM2-31 UPGRADED: Two-Dimensional Magnetic Monopole Gas in Oxide Heterostructures**, ***Ludi Miao***, *Prakash Timsina,* New Mexico State University*; Kyle Shen,* Cornell University

Magnetic monopoles in spin ice emerge as fractionalized excitations of the underlying spin configuration [1]. However, in bulk spin ice, the populations of monopoles and antimonopoles are always equal, resulting in zero net magnetic charge. Here we demonstrate a two-dimensional magnetic monopole (2DMG) gas formed at a spin ice/antiferromagnet (AFM) interface, using Monte Carlo simulation [2]. Unlike the bulk case, this interfacial monopole gas exhibits a non-zero net charge arising from the boundary conditions. We show that a singly charged monopole gas can exist in an AFM/spin ice/AFM sandwich heterostructure, as shown in Fig. 1. Although monopole motion within the spin ice layer costs no energy, the monopoles preferentially accumulate near the AFM/spin ice interface due to entropy maximization [3]. Furthermore, we demonstrate that this charged monopole gas enables novel functionalities: (1) it can be manipulated by external magnetic fields, functioning analogously to a field-effect transistor [2], and (2) engineered monopole traps can store non-volatile magnetic information, with the monopole position serving as a binary state that can be read and written magnetically [4].

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11:20am **PCSI-WeM2-35 Realization of Quantum Size Effects in Rocksalt-Structured MgZnO/MgO Multiple Quantum Wells Grown by Mist CVD**, ***Hiroyuki Aichi***, *Kotaro Ogawa,* Kogakuin University, Japan*; Yukino Abe,* kogakuin University, Japan*; Kyosuke Tanaka, Tomohiro Yamaguchi, Tohru Honda, Takeyoshi Onuma,* Kogakuin University, Japan

Rocksalt (RS)-structured MgZnO alloys have ultrawide bandgap energies up to 7.7 eV. Our group has grown RS-MgZnO epitaxial films by the mist chemical vapor deposition (mist CVD) method. Observation of near-band-edge cathodoluminescence (CL) peak at 187 nm at 300 K paves a way for vacuum ultraviolet light source application. We have developed an alternating precursor supply system to fabricate RS-MgZnO/MgO multiple quantum well (MQW) structures. The MQWs showed smooth surfaces comparable to single layers, and excellent interface flatness and periodicity were confirmed. Present study reports on well thickness dependence to discuss quantum size effects. Magnesium acetate tetrahydrate and zinc acetate dihydrate were used as metal-organic precursors. The Mg molar fraction in source solution was fixed at 0.86. A mixed solvent of deionized water and acetic acid with a volume ratio of 4:1 was used. All layers were grown at 720°C with O_2 carrier and dilution gas flow rates of 4.0 slm and 0.5 slm, respectively. 20-period MQW structures were grown by fixingthe barrier thickness of 10 nm, and by varying the nominal well thicknesses as 0.5, 1, and 3 nm. MQWs show atomically-flat surface morphology with root mean square (RMS) roughness of less than 1 nm. The CL peak energy at 300 K exhibited a distinct blueshift by thinning the well layer thickness. The blueshift is well reproduced by 1D Poisson–Schrödinger calculation. The results indicate the presence of the quantum size effects.

This work was supported in part by Grants-in-Aid for Scientific Research Nos. 25K08495 and 25KJ2089 from MEXT, Japan and The Canon Foundation.

11:25am **PCSI-WeM2-36 Selective Area Growth of PbSe Nanostructures by Molecular Beam Epitaxy**, ***Ashlee Garcia***, *Jarod Meyer, Kira Martin,* Stanford University*; Maksim Gomanko, Sergey Frolov,* University of Pittsburgh*; Kunal Mukherjee,* Stanford University

Selective area growth (SAG) by molecular beam epitaxy of PbSe offers exciting opportunities for integrated photonics and quantum technologies. By using an amorphous mask to define crystal growth, geometric control and deterministic placement of epitaxially smooth nanostructures can be achieved without etching, which can degrade quantum efficiency.[1] Integrating SAG with the advantageous properties of PbSe, including a narrow bandgap, high spin-orbit coupling, low Auger recombination rate, and a desirable defect tolerance,[3-4] could be instrumental for applications such as site-selective quantum dots, nanowire networks, and micro-light-emitting diodes in the mid-infrared. In this work, we explore PbSe SAG and characterize the promising growth morphology and optical quality.

Selective PbSe growth studies were performed over SiO_2 films patterned by e-beam lithography on Si-doped (001) GaAs with a flux supplied by a compound PbSe source equivalent to a growth rate of 0.42 Å/s. Preferred growth of PbSe in the mask openings was observed for substrate temperatures from 345-375°C with no polycrystalline growth on the mask at 375°C. Growth in 100×100nm^2 squares was observed to be largely dominated by one nuclei orientation, producing arrays of well-faceted and ordered squares with low-energy {001} sidewalls at ~365°C, even despite the large lattice mismatch. Atomic force microscopy confirmed smooth surfaces with an average 0.4 nm root-mean-square roughness within individual and 1.3 nm over all grains in Figure 1c. PbSe arrays showed room temperature photoluminescence in the mid-infrared, matching the planar emission wavelength. We aim to understand the structure of the nucleated islands with electron microscopy. This work was supported by the US Department of Energy (DE-SC0019274) and NSF (DMR-1906325).

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11:30am **PCSI-WeM2-37 Ge Quantum Well Structure on Si with Reduced Thickness Using Growth and High-Temperature Diffusion***, **Riis Card**, Jason Dong, Joshua Thompson, Christopher Richardson,* Laboratory for Physical Sciences

The growth of strained Ge quantum wells is of great interest in the fabrication of gate-tunable Josephson junctions. For instance, microwave-frequency superconducting circuits have recently utilized Ge-based Josephson junctions to demonstrate gate-tunable transmon qubits. Historically, the epitaxial growth of high-quality strained Ge on relaxed SiGe buffers has demanded metamorphic growth. To grow a metamorphic buffer with a desired lattice constant at low defect density, microns of material are generally required. Conversely, shrinking total growth thickness is necessary to streamline device fabrication; mesa-etch designs reduce loss from epilayer thickness, but, in its immediate vicinity, a tall mesa structure poses the additional issues of low lithography resolution and irregular deposition thicknesses. In this work, molecular beam epitaxy is leveraged to grow an undoped strained Ge quantum well structure with an over 90% reduction in thickness compared to previous undoped designs.

An alternative heterostructure is presented where 100 nm of Ge has been diffused into an undoped Si (001) substrate wafer to generate a $Si_{0.2}Ge_{0.8}$ virtual substrate. After cooling, growth nominally proceeds with a 100 nm $Si_{0.2}Ge_{0.8}$ buffer, 16 nm strained Ge quantum well, and 22 nm relaxed $Si_{0.2}Ge_{0.8}$ spacer. In a Hall bar, the hole mobility associated with the quantum well exceeds $4.4 \cdot 10^4$ $cm^2/V \cdot s$ with a sheet carrier density of $5.7 \cdot 10^{11}$ cm^{-2} at a temperature of 2 K.

The composition of the $Si_{0.2}Ge_{0.8}$ virtual substrate is verified via an asymmetric reciprocal space map, capturing a distinct SiGe peak and indicating a strained quantum well. Atomic force microscopy reveals that the surface of the sample possesses a leaf-like morphology, closely adhering to the qualities of other anneal-based designs. In this thin heterostructure, a root-mean-square surface roughness of nearly 4 nm suggests that mobility is limited by the roughness of the quantum well interfaces. Further optimization in growth and anneal temperature shall be pursued in order to reduce interface roughness.

11:35am **PCSI-WeM2-38 Investigating the Mechanisms of Remote Epitaxy: Interfaces, Interactions, Nucleation, and Defects***, **Scott Schmucker**, Manny De Jesus Lopez, Sadhvikas Addamane, Quinn Campbell, Ping Lu, Anthony Rice,* Sandia National Labs*; Kevin Jones,* University of Florida*; Justine Koepke,* Sandia National Labs

Remote Epitaxy refers to epitaxial growth on a crystalline substrate coated with a two-dimensional (2D) material. In this process, the epi-layer is oriented to, but not covalently bonded with, the substrate, which facilitates detachment and hetero-integration. This configuration also allows for dynamic rearrangement or “sliding” relaxation at the 2D interface, thereby reducing defects in the epi-layer.

Our results indicate that for the growth of AlN films on SiC substrates, a greater fraction of relaxed AlN is achieved when grown on graphene/SiC compared to AlN grown directly on SiC (Figure 1). However, the success of this epitaxial growth is strongly dependent on the uniformity of a high-quality graphene monolayer on the SiC substrate.

Remote Epitaxy of GaAs and other III-V materials presents different challenges. While SiC has a well-developed graphitization process, high-quality graphene growth on GaAs remains elusive. In the literature, CVD growth of amorphous carbon has been explored as a 2D substitute for graphene. An equivalent fully MBE process has not yet been demonstrated and would enable in situ MBE Remote Epitaxy. We demonstrate epitaxy through amorphous carbon films; however, growth is dominated by pinholes due to film morphology (Figure 2).

To corroborate our experimental results, we employ DFT modeling to elucidate Remote Epitaxy in the context of island sliding energy barriers during the early stages of growth. Additionally, Kinetic Monte Carlo simulations are utilized to assess pinhole defects in 2D materials and evaluate relative contributions of lateral overgrowth versus Remote Epitaxy.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

PCSI
Room Ballroom South - Session PCSI-WeA1
Spin Transport

Moderator: Alex Demkov, The University of Texas

2:00pm **PCSI-WeA1-1 Emergent Spintronic Functionalities in Correlated Oxide Heterostructures**, ***Shinobu Ohya***, The University of Tokyo, Japan **INVITED**

Spintronics promises low-power, multifunctional electronics in which electron spin enables both logic and memory operations. Among the various proposed devices, spin transistors are particularly attractive for non-volatile computing. Key milestones toward their practical realization include the demonstration of large spin-valve effects and the achievement of efficient spin-charge interconversion, both of which are vital for energy-efficient operation. Perovskite oxides provide a versatile materials platform owing to their nearly matched lattice constants, which allow the fabrication of high-quality all-epitaxial heterostructures essential for coherent spin control in devices. These correlated oxides exhibit emergent functionalities, such as two-dimensional transport with strong spin–orbit coupling, metal–semiconductor transitions, topological states, and spin Hall effects, thereby offering unique opportunities for spintronics applications. We first demonstrate a giant planar spin-valve effect in $(La_{0.67},Sr_{0.33})MnO_3$ (LSMO)-based spin-MOSFETs, where oxygen-vacancy engineering creates nanoscale Mott-semiconducting regions, yielding magnetoresistance ratios of ~140% [1] — over two orders of magnitude higher than those of conventional Si-based spin-MOSFETs. Second, we show highly efficient spin-to-charge conversion in the two-dimensional electron gas formed at the strongly correlated $LaTiO_{3+\delta}$ (LTO)/$SrTiO_3$ interface, achieving a record conversion efficiency (referred to as the inverse Edelstein length) of ~190 nm [2]. This performance originates from Rashba spin–orbit coupling combined with reduced spin scattering in correlated metallic LTO. Finally, in the Weyl ferromagnet $SrRuO_3$ (SRO), subtle oxygen-octahedral rotations generate spin Berry curvature that drives spin–orbit torque magnetization switching in a single-layer device [3]. Magnetization reversal occurs at current densities an order of magnitude lower than those required in conventional bilayer systems, without the need for heavy-metal layers. These studies were partly supported by Grants-in-Aid for Scientific Research, ERATO of JST, and the Spintronics Research Network of Japan (Spin-RNJ).[1] T. Endo, S. Ohya *et al*., Adv. Mater. **35**, 2300110 (2023). [2] S. Kaneta-Takada, S. Ohya *et al*., Nat. Commun. **13**, 5631 (2022).[3] H. Horiuchi, S. Ohya *et al.*, Adv. Mater. **37**, 2416091 (2025).

2:40pm **PCSI-WeA1-9 Annealing Effects on the High-Temperature Magnetic Properties of Ta/CoFeB/Ta Films**, *Byeong-Kwon Ju,* ***Hyejin Son***, *Byeongwoo Kang, Ji-Hyeon Kwon,* Korea University, Republic of Korea

Soft magnetic Cobalt–iron–boron (CoFeB) thin films have attracted significant interest for spintronic applications due to its high saturation magnetization and spin polarization. The structural and magnetic properties of CoFeB thin films are strongly influenced by sputtering power [1], post-annealing treatments [2], and variations in CoFeB layer thickness [3]. Spintronic devices operate at elevated temperatures, where thermal effects can alter magnetic damping. Since damping determines switching speed and power consumption, understanding its variation within the operating temperature range is crucial. Most experimental studies of CoFeB films have been limited to room-temperature measurements [4], which cannot provide a systematic understanding of their temperature-dependent damping.

In this study, we investigate the high-temperature magnetic properties of CoFeB thin films with different annealing conditions. Ta (5 nm)/$Co_{20}Fe_{60}B_{20}$ (35 nm)/Ta (3 nm) structures with different annealing conditions (as-deposited, 200 °C, 300 °C, and 400 °C) were measured by ferromagnetic resonance (FMR) spectroscopy at temperatures ranging from 30-160°C to extract the linewidth and resonance magnetic field for dynamic property analysis (Fig. 1). The raw FMR spectra of the 300 °C annealed sample measured at 160 °C showed a monotonic increase in both the resonance field and linewidth with increasing frequency (Fig. 1(a)). The normalized FMR spectra at a fixed frequency of 14 GHz exhibited a gradual increase in both parameters with temperature (Fig. 1(b)). Analysis of the linewidth further showed that the Gilbert damping constant α decreases in the annealed samples compared with the as-deposited film (Fig. 1(c)). The effects of annealing on the high-temperature magnetic response of symmetric Ta/CoFeB/Ta multilayers will be further discussed.

2:45pm **PCSI-WeA1-10 Magneto-Optical Detection of Orbital Hall Effect**, *Kyung-Hun Ko,* Sungkyunkwan University, Republic of Korea*; Daegeun Jo, Peter Oppeneer,* Uppsala University, Sweden*; Hyun-Woo Lee,* POSTECH, Republic of Korea*;* ***Gyung-Min Choi***, Sungkyunkwan University, Republic of Korea **INVITED**

Orbital Hall effect (OHE) refers to the generation of electron orbital angular momentum flow transverse to an external electric field. Theories predict strong OHE in various transition metals of 3d, 4d, and 5d bands [1-3]. In a weak spin-orbit coupling system of 3d metals, OHE can be dominant over spin Hall effect (SHE). To detect OHE, we measured the current-driven orbital accumulation at surfaces of 3d metals of Ti, Mn, and Cu [4-6]. Using the longitudinal magneto-optical Kerr effect (MOKE), we simultaneously detected the in-plane-polarized orbital moments driven by OHE and out-of-plane-polarized orbital moments driven by Oersted field. From the relative comparison of the in-plane and out-of-plane orbital moments, we quantified the magnitude of the OHE-driven orbital accumulation. From the thickness dependence, we distinguished the bulk contribution of OHE and interfacial contribution of orbital Rashba-Edelstein effect (OREE) and determined the orbital diffusion length.

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3:25pm **PCSI-WeA1-18 Anomalous Hall Effect in Co_3PdN Films**, ***Ian Leahy***, *Sita Dugu, Sharad Mahatara, Stephan Lany, John Mangum, Rebecca Smaha, Sage Bauers,* National Lab of the Rockies

Nitride antiperovskites offer a distinct and underexplored playground for uncovering spintronic and magnetic functionalities. Recently, we have synthesized polycrystalline and epitaxial films of phase pure (001) Co_3PdN for the first time. The magnetization behavior of epitaxial films exhibits a 'two-step' magnetization curve that is extremely sensitive to the direction of the applied magnetic field relative to high symmetry directions[1,2]. In Figure 1, we show the magnetic field dependence of the Hall resistivity for fields applied in-plane. In this planar Hall configuration, a clear step-like feature emerges which is dependent on sweep direction, field magnitude, and applied field angle relative to the a-axis. Relatively small, planar magnetic fields generate an anomalous Hall response in Co_3PdN.

By combining MOKE magnetometry and magnetotransport, we identify a rotation of the net magnetization towards the (001) axis (film growth direction) for fields applied in-plane, up to 300 K. We hypothesize that distinct domain dynamics and the magnetic free energy drives the behavior[1,2].The unique tunability of the magnetization combined with a spin-polarized DOS positions Co_3PdN as a potentially powerful spintronics platform.

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PCSI
Room Ballroom South - Session PCSI-WeA2
Oxides III

Moderator: Alessandro Mazza, Los Alamos National Laboratory

4:30pm **PCSI-WeA2-31 Epitaxial Engineering of Emergent Phenomena in Tantalate Perovskites**, ***Kaveh Ahadi***, Ohio State University **INVITED**

Epitaxial tuning knobs, including epitaxial strain, could serve as a powerful parameter that significantly alter the lattice symmetries, affect phase stability, and reshape the energy landscape. In this presentation I will

discuss the epitaxial tuning of tantalate perovskites ($KTaO_3$ and $EuTa_2O_6$) grown using a sub-oxide molecular beam epitaxy method, which we recently developed for tantalates [1]. Next, I will talk about the effect of epitaxial tuning knobs, such as epitaxial strain, on the lattice and electronic structures. Here, I will discuss that$KTaO_3$, a cubic perovskite, can be epitaxially strained into a highly tunable ferroelectric. $KTaO_3$ films, grown commensurate to $SrTiO_3$ (001), experience an in-planecompressive strain of -2.1 % that transforms the otherwise cubic structure into atetragonal polar phase with a transition temperature of 475 K, consistent with ourphase-field calculations. The Curie temperature and the spontaneouselectric polarization are systematically controlled with epitaxial strain. Scanning transmission electron microscopy reveals cooperative polar displacements of thepotassium columns with respect to neighboring tantalum columns at room temperature. Optical second harmonic anisotropic rotation results are described by a tetragonal polar point group (*4mm*), indicating emergence of a global polar ground state.

Finally, I discuss our recent results on epitaxial control of ordering in fractionally occupied double perovskite, $EuTa_2O_6$ [2]. The intrinsic crystal anisotropy of $EuTa_2O_6$ plays a pivotal role, underscoring how targeted structural modifications can facilitate the emergence of novel quantum states. The crystal and electronic structures of $EuTa_2O_6$ are investigated. X-ray diffraction and electron microscopy reveal the layered *A*-site ordering. Angle-resolved photoemission spectroscopy, along with density functional theory calculations, provide direct insight into the electronic structure, unveiling the potential for engineered confined states within bulk materials. These findings highlight $EuTa_2O_6$ as a platform for studying 2D-like electronic phenomena in a 3D context, paving the way for novel device architectures.

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5:10pm **PCSI-WeA2-39 Pockels Effect in Single-Domain a-Oriented BaTiO3 on Vicinal Si (001)**, ***Jason Tischler,*** University of Texas at Austin*; Agham Posadas,* La Luce Cristallina*; David Smith,* Arizona State University*; Kamyar Barakati, Kalinin Sergei,* University of Tennessee Knoxville*; Alexander Demkov,* University of Texas at Austin

Silicon (Si) integrated photonics is an emerging technology developed for the communications industry with emerging applications in quantum and neuromorphic computing [2, 3]. These devices provide advantages in data transmission rates by modulating optical signals in Si waveguides. However, Si by itself is a poor modulator of light as it has no intrinsic electro-optic effect. Barium titanate (BTO) demonstrates a large electro-optic response known as the Pockels effect due to it being a non-centrosymmetric medium. The Pockels effect is the change in refractive index of the material due to an external electric field. This response is described by a tensor and the largest component for BTO is r_{42}, which is reported to be 1,300 pm/V in bulk [4], and 923 pm/V in thin films [5,6]. To access this large value in a waveguide phase-shifter, one uses thin BTO films with the so-called a-axis orientation [7]. When BTO is epitaxially grown on Si (001) in the a-axis orientation, meaning the long c-axis is in-plane, two orthogonal in-plane crystallographic domains form. This creates problems in the form of Rayleigh scattering at the domain boundaries and not being able to fully utilize the high r_{42} coefficient.

In this talk we demonstrate the use of a 4° miscut vicinal Si (001) substrate to stabilize a single in-plane orientation growth of a-axis BTO on strontium titanate (STO) buffered Si by molecular beam epitaxy (MBE). In this study, utilizing x-ray diffraction (XRD) techniques and scanning transmission electron microscopy (STEM), we detail the crystalline microstructure confirming a single in-plane BTO orientation; The ferroelectric domain structure is characterized using piezo-force microscopy (PFM) and the electro-optic response is probed via transmission geometry Pockels measurements.

5:15pm **PCSI-WeA2-40 Epitaxial Single Crystal MgO Buffers on Si (100)**, ***Pablo Espinosa Argaiz,*** *Alexander Demkov,* University of Texas at Austin

The integration of functional metal oxides with silicon has been a persistent challenge due to the thermodynamic instability of their resulting interfaces [1]. Crystalline oxide buffer layers have been used as a solution by providing a thermodynamically stable transition layer. Magnesium oxide (MgO) buffers have been shown to work as effective pseudo-substrates for metal oxide epitaxy [2, 3], and its deposition on silicon has been shown to be stable [4].

In this talk we report an extensive study of high-quality MgO buffer layers using molecular beam epitaxy (MBE) on Si(100) substrates. The buffers were grown through electron-beam evaporation of single crystal MgO, which was deposited at 300°C under an oxygen partial pressure of $3.7x10^{-5}$ Torr. The reflection high-energy electron diffraction (RHEED) pattern (Figure 1.a) reveals a modulated pattern along the MgO[100] direction, indicating the beginning of small island formation and surface faceting. The thickness dependence on the films' crystallinity was studied through the FWHM of the (200) MgO Bragg peak rocking curve as seen in Figure 1.b. The trend suggests an improvement in the crystallinity as the layers become thicker. Figure 1.c shows the scanning transmission electron microscopy (STEM) image of a cross section of the MgO/Si interface, revealing an in-plane epitaxial relationship of MgO <100> || Si <100> with a 4:3 coincident site arrangement between the MgO and Si conventional unit cells. The figure also reveals the presence of tilted MgO grains and small-angle grain boundaries. The interface layer observed in Figure 1.c was investigated using x-ray photoelectron spectroscopy (XPS), suggesting the formation of Mg-O-Si bonds at the interface. Additionally, the measured band alignment at the MgO/Si interface and its relation to first principles calculations of various interface models will be discussed.

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5:20pm **PCSI-WeA2-41 Plasma-Induced Surface Modification of Indium for Improved Bonding**, ***Kristen Steffens,*** *Sujitra Pookpanratana, Junyeob Song, Marcelo Davanco, Tammy Lucas, John Biesecker, Daniel Schmidt,* National Institute of Standards and Technology (NIST)

Bonding plays an important role in advanced microelectronics integration and packaging by bringing together components and devices produced separately.Surface-pretreatments on bonding materials have been consistently found to be crucial to achieving a high-quality bond, despite incomplete understanding of why certain treatments have greater success than others.Our project aims to improve understanding of some of these bonding pre-treatment effects to provide information to enable more efficient development of bonding protocols.

Indium is a critical material for conductive contacts in the fabrication of cryogenic low-temperature electronics and optical detectors for infrared and microwave applications, because In is a superconducting material which retains its ductility and adhesion properties during thermal cycling.Certain pre-bond plasma treatments increase the success of In-In bond adhesion.We have observed that plasma chemistries such as H_2/He, which do not include N_2 as a plasma gas, promote more successful In-In bonding.To understand why, we investigate the effects of atmospheric plasma exposure on In surfaces for several plasma chemistries including $He/H_2/N_2$, He/H_2 and He/N_2.X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) are used to characterize In surfaces prior to and after ambient pressure plasma treatment.All plasma treatments decreased the amount of carbon and increased the amount of In-oxide present when compared to an untreated film.N_2-containing plasmas resulted in the appearance of an additional high binding energy peak in the N 1s XPS spectrum.We postulate that this may be due to nitrate species formed on the In native oxide surface. Additional experiments are planned to assess the plausibility of this explanation.In foil was measured prior to and after Ar sputter cleaning for comparison to treated samples.

UPS measurements showed that all plasma chemistry treatments lowered the work function compared to the non-treated control.Greater spatial variation in work function was observed for chemistries with high N_2 versus those with little to no N_2.This finding possibly correlates with poorer bonding for N_2 containing plasmas.

5:25pm **PCSI-WeA2-42 High-Temperature Resilient Neuromorphic Device based on Optically Configured Monolayer MoS2 for Cognitive Computing**, ***Pukhraj Prajapat,*** *Govind Gupta,* National Physical Laboratory, India

High-temperature neuromorphic devices are becoming more and more essential as technology progresses to support space exploration and survive extreme conditions such as those found in factories. To overcome this need, the researchers are devising technologies that imitate human brain structure and operation. In this work, we present a scalable neuromorphic

device based on a monolayer of MoS_2, that demonstrates operation at 100°C. The device portrays excellent electrical performances mostly due to the great thermal stability of monolayer MoS_2 and its mechanical flexibility. Among these performances are low power consumption, fast switching, high resistance ratio, low switching voltage, and long stable endurance (~10^3 cycles). Besides, the device mimics neuromorphic behavior by embedding the synaptic plasticity that is the major functional property of biological neural networks, thus allowing advanced cognitive computing in extreme environments. This is the first step toward a combination of materials science and neuromorphic computing, and it clears the way for smart resilient electronics that could survive in a variety of harsh conditions. This research is targeting a major change in the area of high-temperature electronics, and this progress is paving the way for obtaining future high-performance electronics that can meet the needs of modern technology.

5:30pm **PCSI-WeA2-43 Understanding Dielectric Breakdown Using EDMR and NZFMR**, ***Colin McKay***, Sandia National Laboratories*; George Bodenschatz, Kaila Burges, Elijah Allridge, Michael Elko, Patrick Lenahan,* Penn State University*; David Hughart, Gaddi Haase,* Sandia National Laboratories

Time dependent dielectric breakdown (TDDB) is a fundamental problem in solid state electronics which is still not fully understood. Different models in the literature provide very different expected lifetimes. A deeper understanding of the physical mechanisms of TDDB can be gained from using electrically detected magnetic resonance (EDMR) and near zero field magnetoresistance (NZFMR). This abstract shows data from such a study. We report a fundamental advance in our understanding of TDDB in SiO_2 and the first direct observation of the generation of a specific point defect, the E' center, due high field gate stress using EDMR, NZFMR, and other techniques at room temperature. EDMR and NZFMR are spectroscopic techniques sensitive only to electrically active defects.

In this study, gate oxides in large arrays of silicon on insulator (SOI) n-MOSFETs were subjected to high electric field stress at 7.5V. Damage caused by the stress was characterized using the Fitzgerald-Grove gated diode method, capacitance vs voltage (CV), EDMR, and NZFMR measurements. The gate oxides were 7 nm thick and the gate areas of the transistor arrays were between 5,000 μm^2 and 50,000 μm^2.The early increase in peak DCIV current indicates that the first stage of damage is characterized by interface state generation, specifically Pb centers, with no appreciable increase in bulk oxide defects. The generation of interface states is accompanied by the redistribution of hydrogen away from recombination centers shown by the NZFMR results. The interface state density eventually starts to saturate, followed by an increase in bulk oxide defects, specifically E' centers, represented by a shift in the voltage of the DCIV peak current. The Pb and E' centers were identified via their EDMR signals. The E' spectrum only appears after long stress durations. This new understanding of the different stages of damage provides a fundamental insight into the physics of damage mechanisms during the leadup to TDDB.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

5:35pm **PCSI-WeA2-44 Interfacial Polarization in Polymer-Based Dielectric Composites with 2d Nanomaterials**, *So-Yeon Jun,* ***SeGi Yu***, Hankuk University of Foreign Studies, Republic of Korea

The dielectric behavior of polymer-based composite films was systematically investigated with a particular focus on the interfacial polarization phenomena arising from the incorporation of conducting two-dimensional (2D) nanoplatelets. Ferroelectric $BaTiO_3$ (BTO) nanoparticles were employed as a primary filler; while MXene, graphene oxide (GO), and reduced GO (rGO) served as co-fillers to modulate the interfacial effects. Cyanoethyl pullulan (CEP) was used as a polymer matrix due to its high dielectric behavior among polymers. A reference sample, containing BTO nanoparticle fillers only in a CEP matrix, was also prepared to isolate the contribution of the 2D nanomaterials, which resulted in four dielectric composite samples. MXene platelets were delaminated in dimethyl sulfoxide (DMSO) via ultrasonication for 2 hours, and rGO was chemically reduced from GO using hydrazine over 8 hours—both conditions optimized in prior studies [1,2] to enhance dielectric performance. All components were dispersed in dimethylformamide (DMF) and spin-coated onto ITO substrates to form uniform dielectric films.

The incorporation of conducting 2D nanoplatelets significantly enhanced the dielectric constant of the composites. The highest value was achieved with the MXene-incorporated film (~200 at 1 kHz), followed by GO films (~130) and rGO films (~120), all substantially higher than the reference film containing BTO only (~90). However, this enhancement was accompanied by an undesirable increase in the dielectric loss (tan δ) due to percolative linkage of fillers. The loss increased, from 0.048 for the reference sample, to 0.053 for GO, 0.10 for MXene, and 0.22 for rGO, respectively.The observed dielectric enhancement is attributed to pronounced interfacial polarization at the filler-matrix boundaries, facilitated by the high aspect ratio and conductivity of the 2D nanoplatelets. Among them, MXene demonstrated superior interfacial coupling due to its metallic conductivity, leading to more effective charge accumulation at interfaces. In addition, MXene can successfully suppress the increase in the dielectric loss which is difficult to control for nanomaterial incorporation within a polymer matrix. Raman spectroscopy and X-ray photoemission spectroscopy (XPS) analyses corroborated the structural and electronic characteristics responsible for these effects. These findings demonstrate the critical role of interfacial polarization in tailoring the dielectric properties of polymer-based composites and suggest that MXene-based systems hold promise for next-generation electronic and energy storage applications, where high permittivity and controlled loss are essential.

5:40pm **PCSI-WeA2-45 Switchable Electron-Phonon Scattering Strength in Monolayer Hexagonal Boron Nitride**, *Alv Johan Skarpeid,* University of Oslo, Norway*; Noah Joseph Hourighan,* Graz University of Technology, Austria*; Richard Justin Schenk,* University of Oslo, Norway*;* ***Håkon Ivarssønn Røst***, University of Bergen, Norway*; Giovanni Di Santo, Luca Petaccia,* Elettra-Sincrotrone Trieste, Italy*; Bodil Holst,* University of Bergen, Norway*; Anton Tamtögl,* Graz University of Technology, Austria*; Justin William Wells,* University of Oslo, Norway

In the past decade, the layered compound hexagonal boron nitride (hBN) has drawn considerable attention due to its compatibility with various low-dimensional van der Waals (vdW) materials [1]. While hBN resembles graphene in lateral size, crystalline structure, and Debye frequency, its two distinct sub-lattices give rise to a significant energy band gap between the valence and conduction bands [2]. Recently, it was predicted that hBN should host strong electron-phonon coupling (EPC) in its electronic π- and σ-bands [3], reminiscent of the reported (and debated) interactions in the graphene σ-bands [4]. Since then, we have confirmed this EPC from observable energy renormalizations in the hBN band structure [5].

We will showcase the electron-phonon coupling (EPC) in hBN, highlighting how changing the substrate interaction, e.g., by adatom intercalation, can influence coupling strength (see Fig. 1). By combining angle-resolved photoemission and neutral helium atom scattering, we will demonstrate how these techniques together help demystify the scattering modes involved in electron-hole recombination. We will also mention the broader implications of EPC in materials with finite electronic band gaps.

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5:45pm **PCSI-WeA2-46 Epitaxial Growth of Superconducting $CoSi_2$ for Advancements in Quantum Information Sciences**, ***Julian Choi***, *Teun van Schijndel, Yu Wu, Christopher Palmstrom,* University of California Santa Barbara

Josephson junctions (JJs) are superconductor/insulator/superconductor structures crucial in superconducting quantum circuits due to their non-linear inductance creating an anharmonic oscillator that can be used as a qubit. They are often created using amorphous materials. The amorphous oxide and its interfaces with the superconductor are believed to result in two-level energy loss systems that limit performance. One way to progress in this field is to carefully select materials that best minimize this loss. In this context, $CoSi_2$ is particularly interesting for these systems because it has the potential to be fully epitaxial with silicon, thus eliminating any amorphous materials. This is due to the capability of growing a single crystalline Si barrier on $CoSi_2$, which is possible because of their similar crystal structures and small lattice mismatch of approximately 1.2% [1].In this talk, we demonstrate the Si substrate preparation and epitaxial growth of superconducting $CoSi_2$ by molecular beam epitaxy (MBE). We systematically investigate the crystalline structure, topography, and superconducting properties of the resulting films. The reflection high-

energy electron diffraction (RHEED) patterns after the cleaning process exhibited Laue arcs, indicating an oxide-free and smooth surface. During the growth, Co is deposited and $CoSi_2$ is formed through reaction with the Si substrate heated to at least 200 C. 2 x 2 diffraction patterns are visible in RHEED, which indicate epitaxial growth, later confirmed by high resolution X-ray diffraction (XRD). Atomic force microscopy (AFM) shows grain formation on the surface and measurements using an adiabatic demagnetization refrigerator show the superconducting transition temperature (T_c) of the $CoSi_2$ film as 0.58 K, which is lower than the bulk value of 1.4 K [2]. This T_c reduction suggests that the film is too thin or may not be completely single crystalline. We then investigate the growth of $CoSi_2$ films at different temperatures, evaluate the impact of post-growth anneals, and determine how these factors influence their superconducting properties.

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5:50pm **PCSI-WeA2-47 Interfacial Oxidation in Niobium Films Probed by HAXPES*, Ananya Chattaraj,*** Brookhaven National Laboratory

Niobium (Nb) thin films are widely used in superconducting quantum circuits owing to their relatively high superconducting transition temperature (T_c) and compatibility with microfabrication processes [1,2]. Device performance, however, is often limited by dielectric losses originating from interfacial oxides in which two-level systems introduce parasitic energy dissipation [2,3]. A deeper understanding of the structural and chemical evolution of Nb oxides, as well as their depth distribution, is therefore critical for improving thin-film quality and coherence in superconducting devices. In this presentation we demonstrate the deposition of Nb thin films using DC magnetron sputtering. The oxidation behavior and interfacial chemistry of the films were investigated using laboratory-based X-ray photoelectron spectroscopy (XPS) together with variable-photon-energy Hard X-ray Photoelectron Spectroscopy (HAXPES) performed at the NSLS-II synchrotron. HAXPES measurements spanning photon energies from 2000–5500 eV enabled non-destructive, depth-resolved analysis from the surface oxide to the metallic Nb bulk. Quantitative fitting of the Nb 3d and O 1s core-level spectra revealed multiple suboxide species (Nb_2O_5, NbO_2, and NbO_x) and their gradual evolution across the Nb/NbO_x interface [2,4]. The variable-energy approach provided nanometer-scale insight into oxidation gradients and interfacial structure that are inaccessible to conventional XPS, highlighting the power of synchrotron-based depth profiling for complex superconducting thin films. Electrical transport measurements confirmed a T_c of approximately 9 K, demonstrating that high-quality superconducting properties can be achieved using sputtered Nb growth. The integrated structural, spectroscopic, and transport characterization establishes a framework for understanding interfacial oxidation mechanisms in Nb thin films and provides guidance for mitigating oxide-related losses in superconducting and quantum device technologies.

[1] Joshi et al Physical Review Applied. 2023 Aug 1;20(2):024031.

[2] Murthy et al. ACS nano. 2022 Sep 26;16(10):17257-62.

[3] Verjauw et al. Physical Review Applied. 2021 Jul 1;16(1):014018.

[4] Burnett et al. arXiv preprint arXiv:1512.02553.

5:55pm **PCSI-WeA2-48 Room Temperature Electrically Detected Magnetic Resonance of Performance Limiting Defects in GaN Pn Junction Diodes*, Dustin T. Hassenmayer, Patrick M. Lenahan, M.J. Elko,*** Penn State University*; David A. Fehr, Michael E. Flatte,* University of Iowa*; B.R. Tuttle,* Penn State University*; R. Chu, Yuxin Du,* University of Illinois at Urbana-Champaign

In order to utilize any semiconductor material, it is important to understand the physical and chemical nature of its most important electrically active defects. Multiple studies have been reported on defects in GaN but direct experiment evidence linking specific defect structures to their properties is very limited. Electrically detected magnetic resonance (EDMR) along with conventional electron paramagnetic resonance (EPR) has unrivaled analytical power for identifying point defects. However, EDMR has many orders of magnitude greater sensitivity than conventional EPR [1-2]. In this work, we report on the EDMR detection of an important defect in GaN devices with detailed observation of hyperfine structure. These observations involve room temperature EDMR measurements of GaN pn diodes. The measurements involved device active region of <10-7 cm3. There have been longstanding sensitivity barriers which have limited the application of magnetic resonance techniques on III-V materials. This work may have cleared a path to identifying point defects in a variety of III-V devices. The first and second derivative EDMR signal shown in figure 1 was obtained on a GaN pn junction diode at room temperature with 3.05 V forward bias ($B \perp c$). The EDMR signal has a $g \approx 2.005$, and a rich, partially resolved hyperfine structure consisting of 10 lines. These are the first reported room temperature EDMR or EPR results reported on GaN devices. In figure 1, we show a model calculation involving an unpaired electron shared with three equivalent Ga nuclei with 60% 69Ga and 40% 71Ga and a hyperfine coupling constant of 32.1 G and 44.4 G, respectively. The hyperfine structure is similar to the previously observed L1 center in undoped GaN irradiated by 2.5 MeV electrons reported by Watkins et al. [3].

PCSI

Room Ballroom South - Session PCSI-ThM

Quantum Materials

Moderator: Kirstin Alberi, National Renewable Energy Laboratory

8:30am **PCSI-ThM-1 Correlated Electron States in Multilayer Graphene: From Superconductivity to Half-Integer Quantum Hall Effects**, ***Mark Bockrath,*** Ohio State University **INVITED**

Thin graphite flakes behave as two-dimensional conductors in sufficiently high magnetic fields, with quantum Hall states extended throughout the bulk of the flake for low doping, and confined to the surfaces for large doping. I will discuss our observation of half-integer fractional quantum Hall states at large total filling factors. These single-component states likely stem from Pfaffian wavefunctions derived from those in graphene bilayers, which are predicted to host nonabelian quasiparticles. The facile integration of graphite with top and back surface gates makes this an excellent system to explore device geometries capable of manipulating such quasiparticles. Moreover, the group velocity v_F of the electrons in a flat band superconductor is extremely slow, resulting in quenched kinetic energy. Superconductivity thus appears impossible, as conventional theory implies a vanishing superfluid stiffness, coherence length, and critical current. Using twisted bilayer graphene (tBLG), we explore the profound effect very small v_F in a superconducting Dirac flat band system. We find an extremely slow $v_F\sim$ 1000 m/s for filling fraction between -1/2 and -3/4 of the moiré superlattice. This velocity yields a new limiting mechanism for the superconducting critical current, with analogies to a relativistic superfluid. We estimate the superfluid stiffness, which determines the electrodynamic response of the superconductor, showing that it is not dominated by the kinetic energy, but by the interaction-driven superconducting gap, consistent with recent theories on quantum geometric contributions. Finally, we have shown that incompressible states form at 1/3 fractional filling factors in twisted bilayer graphene at angles larger than the magic one that are strongly dominant over integer fillings. These results are in agreement with a strong-coupling theory based on Coulomb interactions between electrons occupying three-lobed Wannier orbitals, leading to novel symmetry-broken phases with distinct charge, spin, and valley order.

9:10am **PCSI-ThM-9 Surface Passivation in Black Phosphorous/GaAs Ultra-Thin Heterojunctions**, ***Peter-Jonas Ela,*** *Francesca Cavallo, Emma Renteria,* University of New Mexico*; Sadhvikas Addamane,* Sandia National Laboratories

This work focuses on investigating process-structure-property relationships in bP/GaAs ultrathin heterojunction photodiodes, which are excellent candidates for radio-frequency-hard detection of visible-to infrared waves. In particular, the subject of the study is the effect of bP oxidation on the leakage current of the device.

9:15am **PCSI-ThM-10 Electronic and Optical Properties of Lanthanide-Doped MoS_2: Impact of Ionic Size and Orbital Configuration Mismatch**, ***Hyosik Kang,*** *Lukas Muechler,* Penn State University

Single-photon emitters (SPEs) are crucial for quantum technologies such as quantum simulation, secure quantum communication, and precision measurements. Two-dimensional transition-metal dichalcogenides (TMDCs) provide an attractive platform for SPEs due to their atomically thin structure, high extraction efficiency, and compatibility with chip-based photonic devices. However, conventional TMDC SPEs emit mainly in the visible range, which limits their use for telecommunication applications that require infrared wavelengths. Lanthanide doping in TMDCs, such as MoS_2, offers a potential solution by introducing sharp, *f* orbital-derived emissions in the infrared range. Yet, the feasibility and impacts of introducing these dopants remain uncertain due to the large ionic radii of the lanthanides.

In this context, we employ density functional theory calculations to investigate the structural, electronic, and optical impact of lanthanide-doped MoS_2 monolayers (Ln=Ce, Er). By evaluating formation energies with adjacent S vacancies, we assess that sulfur vacancies adjacent to Ln sites play a key role in mitigating lattice strain, enabling thermodynamically stable lanthanide incorporation. Charge-state and band structure analysis reveal that *f* orbital-derived defect states and additional host-related states emerge near the band gap, originating from the mismatch of the orbital configuration between the dopant and the host lattice. Furthermore, optical absorption analysis reveals multiple defect- and *f* orbital-related transitions within the band gap range of the host material. Notably, Er_{Mo} exhibits sharp, weak *f-f* optical transitions (0.9-1.1 eV), suggesting the feasibility of defect engineering for SPE. In contrast, Ce_{Mo} shows only defect-related absorption due to its empty *f* shell.

9:25am **PCSI-ThM-12 Band-Bending in Dirac Semi-Metal/Semiconductor Interfaces**, ***Anthony Rice,*** *Ian Leahy, Kirstin Alberi,* National Lab of the Rockies

Cd_3As_2 provides an excellent platform for studying the properties Dirac semi-metals. Electrically, it has a single band crossing well isolated from trivial bands, with an Fermi level that is intrinsically close to the Dirac point. Additionally, its similarity structurally and chemically with III-V and II-VI compounds allow for straightforward combination with semiconductors, creating pathways for high-quality epitaxial integration to utilize the unique properties of topological semimetals. Beyond their stand-alone properties, due to their vanishing density of states near Dirac points, large shifts in the Fermi level may occur from band-bending, creating possibilities for unique charge control at interfaces with implications for devices and even contact layers.

Here, Cd_3As_2/n-GaAs interfaces are first explored. Using molecular beam epitaxy, Cd_3As_2 layers are grown directly on GaAs. Depending on the doping, these Cd_3As_2 layers have a Fermi level 30-100 meV above the Dirac point. Using capacitance-voltage measurements, band alignments are calculated, suggesting a mid-gap alignment of the Dirac point. Due to the large dielectric constant of Cd_3As_2, most of the built-in voltage drop occurs in the n-GaAs layer, giving rise to a Schottky barrier. Attempts at forming rectifying barriers on p-GaAs have resulted in Ohmic junctions, suggesting band-bending in the Cd_3As_2 layer results in the near-interface region becoming p-type. Results with p-CdTe will also be discussed.

9:30am **PCSI-ThM-13 Angle Dependent Magnetoresistance in Cd_3As_2 Thin Films**, ***Ian Leahy,*** *Anthony Rice,* National Lab of the Rockies*; Herve Ness,* Department of Physics, King's College London, UK*; Jocienne Nelson, Mark van Schilfgaarde, Kirstin Alberi,* National Lab of the Rockies

Measurements of the magnetic field angle dependence of magnetotransport have become very popular in the study of topological semimetals, potentially containing information about Fermi surface anisotropy, magnetocrystalline anisotropy, or mobility anisotropy[1-3]. Here, we report on a detailed analysis of angle dependent magnetotransport in (001) Cd_3As_2 thin films of varying carrier densities. We identify a range of possible behaviors depending on mobility and carrier density. Most strikingly, we find a large, positive magnetoresistance (MR) for both and (black trace in Fig. 1), contingent on the direction of the applied current and sample carrier density. In the configuration, this large MR can evolve from negative longitudinal MR at low magnetic fields. Using an 8 x 8 model in a magnetic field and linear response theory, we calculate the theoretical field angle and field magnitude dependence of the longitudinal and Hall resistivities, finding nontrivial dependence on the Fermi energy, which we compare to our experimental results.

[1] A. Collaudin, B. FauquAngle, Y. Fuscya, W. Kang, and K. Behnia, *Angle Dependence of the Orbital Magnetoresistance in Bismuth*, Physical Review X, 5, 021022 [https://journals.aps.org/prx/pdf/10.1103/PhysRevX.5.021022] (2015).

[2] J. Wang, H. Yang, L. Ding, W. You, C. Xi, J. Cheng, Z. Shi, C. Cao, Y. Luo, Z. Zhu, J. Dai, M. Tian, and Y. Li, *Angle-dependent MR and its implications for Lifshitz transition in W_2As_3*, npj quantum materials, 4, 58 [https://www.nature.com/articles/s41535-019-0197-5] (2019).

[3] S. Ghosh, A. Low, N. Devaraj, S. Changdar, A. Narayan, S. Thirupathaiah, *Extremely large and angle dependent MR in Kagome Dirac Semimetal RFe_6Sn_6 (R = Ho, Dy)*, Journal of Alloys and Compounds, 1040 183506 [https://www.sciencedirect.com/science/article/pii/S0925838825050674] (2025).

10:00am **PCSI-ThM-19 Atomic-scale identification of Boson Complexes across Heterogenous Interfaces in 2D Materials**, ***Kory Burns,*** University of Virginia, USA*; Hayden Barry,* University of Virginia*; Christopher Smyth,* Sandia National Laboratories, USA*; Jordan Hachtel,* Oak Ridge National Laboratory, USA **INVITED**

Two-dimensional (2D) compound semiconductors exhibit a range of levels of disorder dependent on their stoichiometry, which can be engineered based on growth conditions, substrate interactions, or atom-by-atom modifications with charged projectiles. There is an entire framework of studies that builds upon research dedicated towards the associated properties with heterogeneities in films, but fail to make one-to-one correlations with the atomic arrangement of the lattice and the

optical/infrared emissions. In this talk, we first use aberration-corrected scanning transmission electron microscopy (STEM) to visualize the atomic sites and interfacial growth along semiconducting films. Then, monochromated electron energy loss spectroscopy (EELS) inside an aberration-corrected STEM is used, which greatly reduces the energy distribution of the electron source to maximize the energy resolution without sacrificing too much spatial resolution. Accordingly, we map the high-frequency vibrational modes and exciton complexes in transition metal dichalcogenides (TMDs) moiré structures (Fig. 1) and transition metal monochalcogenides (TMCs) lateral interfaces (Fig. 2). We strategically incorporate off-axis EELS into our workflow, in which it suppressed delocalized responses from Cherenkov radiation losses, to correlate the impact single atom modifications have on the vibrational and optical spectrum. Ultimately, we address applications ranging from magnetic-tunnel transistors to energy harvesting devices.

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