

PCSI

Room Ballroom - Session PCSI-SuA

Magnetism, Altermagnets, & Spin Phenomena

Moderator: Matthew Brahlek, Oak Ridge National Laboratory

3:30pm **PCSI-SuA-1 Controlling Magnetism in RuO₂ through Strain and Surface Engineering**, *Jong Seok Lee*, Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea

INVITED

Altermagnetism has recently emerged as a distinct class of magnetic order that combines key characteristics of ferromagnets and antiferromagnets. Its compensated antiparallel spin structure, intertwined with crystallographic rotational symmetry, gives rise to momentum-dependent spin splitting and unconventional magnetic responses, offering new opportunities for next-generation spintronic applications. Despite these intriguing properties, direct observation and control of the altermagnetic order remain challenging. In particular, the magnetic ground state of RuO₂, one of the most intensively studied candidate altermagnets, remains under active debate due to conflicting experimental observations.

In this presentation, I will discuss two complementary approaches to stabilizing and controlling altermagnetism in RuO₂: anisotropic strain engineering in thin films and chemical modulation of surface electronic states. In epitaxial RuO₂ films, anisotropic strain provides a means to modify the structural and electronic environment governing magnetic order, enabling control of the altermagnetic state. Beyond strain engineering, carrier doping offers another route to stabilizing compensated magnetic order. We show that modification of the surface chemical state of RuO₂ can induce a distinct surface magnetic state while leaving the bulk largely unaffected. Surface-sensitive X-ray photoemission spectroscopy, optical second-harmonic generation, and Kerr effect imaging reveal pronounced temperature-dependent changes and domain formation in oxygen-containing-species-modified RuO₂, in clear contrast to stoichiometric RuO₂. These observations indicate the emergence of surface magnetism associated with chemically induced electronic modulation. Together, our results demonstrate that both lattice strain and surface electronic engineering provide effective pathways for manipulating magnetism in RuO₂, highlighting the importance of structural and electronic degrees of freedom in understanding its debated magnetic ground state and providing new opportunities for nanoscale altermagnetic spintronics.

4:00pm **PCSI-SuA-7 UPGRADED: Molecular Beam Epitaxy of Hybrid Heterostructures Interfacing an Altermagnet (CrSb) with a 2D Ferromagnet (CrTe₂) and a Topological Insulator (Sb₂Te₃)**, *Sandra Santhosh, Kalana Halanayake, Soumyanil Adhikary, Supriya Ghosh, Anthony Richardella, Danielle R. Hickey, K. Andre Mkhoyan, Nitin Samarth*, Pennsylvania State University

Altermagnetism is a theoretical classification of magnetic materials exhibiting a unique coexistence of long range antiferromagnetic order and non-relativistic spin-polarized electronic band structure. NiAs-type CrSb in the bulk is theoretically and experimentally categorized as a metallic altermagnet at room temperature with g-wave symmetry. We recently reported the molecular beam epitaxy (MBE) of thin films of epitaxial CrSb on insulating SrTiO₃(111) substrates via a buffer layer of topological Sb₂Te₃, using angle resolved photoemission spectroscopy (ARPES) and polarized neutron reflectometry to verify the altermagnetic nature of these films [1]. Here, we discuss a detailed comparison of the MBE growth of CrSb on insulating SrTiO₃(111) using two different buffer layers, Sb₂Te₃ and CrTe₂. Reflection high energy electron diffraction, X-ray diffraction, and transmission electron microscopy confirm the epitaxial growth of good quality films of NiAs-type CrSb (0001) in both cases. We also use *in vacuo* angle resolved photoemission spectroscopy at room temperature to verify the g-wave symmetric altermagnetic band splitting in 10 nm thick CrSb films grown on both types of buffer layers. *Ex situ* transport measurements reveal the absence of an anomalous Hall effect at room temperature, as expected theoretically from a g-wave altermagnet without additional broken symmetry. We discuss how the synthesis of these hybrid heterostructures that interface a room temperature altermagnet with topological insulators and 2D magnets provides a promising platform for novel spintronics devices.

Acknowledgements

This work is supported by the Penn State Two-Dimensional Crystal Consortium-Materials Innovation Platform (2DCC-MIP) under NSF Grant No. DMR-2039351 and the Penn State MRSEC Center for Nanoscale Science via NSF award DMR 2011839.

References

1. S. Santhosh *et al.*, *Adv. Mater.* **37**, e08977 (2025)

4:15pm **PCSI-SuA-10 First- Principles Study of Strain- Controlled Magnetism in MnBi₂Se₄ Heterostructure**, *Narendra Phulara*, University of Kansas, Nepal

Abstract :We present a first-principles study of the magnetic ground state of the magnetic quantum material MnBi₂Se₄ supported on a ferroelectric substrate. Using density functional theory, we will first compare ferromagnetic and antiferromagnetic configurations of freestanding MnBi₂Se₄. We will then obtain a fully relaxed slab structure of the ferroelectric substrate, construct the MnBi₂Se₄/substrate heterostructure, and determine its equilibrium geometry and magnetic ground state. Finally, shear strain will be applied to the relaxed heterostructure to examine how structural deformation modifies the relative stability of the ferromagnetic and antiferromagnetic states. This systematic study will establish whether shear strain provides an effective route for controlling the magnetic ground state of MnBi₂Se₄ in ferroelectric-based heterostructures for potential spintronic applications.

4:20pm **PCSI-SuA-11 Investigating Magnetocaloric Properties of NdGaO₃**, *Gabriel Ruiz Ruiz*, Los Alamos National Laboratory

NdGaO₃ is a rare-earth perovskite oxide that undergoes antiferromagnetic ordering below ~1.2 K. It is widely used as a substrate for the epitaxial growth of high-quality high-temperature superconducting thin films, including cuprates and the recently discovered nickelates. However, the intrinsic magnetic and magnetocaloric properties of the substrate can significantly influence measurements of these superconductors, particularly in high magnetic fields under adiabatic conditions, such as those employed at the pulsed Field Facility of National High Magnetic Field Laboratory (NHMFL). To evaluate the role of the substrate, we investigated the low-temperature magnetic and magnetocaloric properties of NdGaO₃ through magnetization measurements.

We observe clear antiferromagnetic ordering below 1.2 K and a large magnetic entropy change arising from field-induced suppression of magnetic disorder. These results demonstrate that NdGaO₃ exhibits a pronounced magnetocaloric effect at low temperatures. Consequently, the substrate can undergo substantial temperature changes during pulsed-field experiments, potentially affecting the measured response of superconducting nickelate thin films. These findings underscore the importance of accounting for the magnetocaloric behavior of NdGaO₃ when interpreting low-temperature, high-field measurements of superconducting heterostructures. With this research we strive to extract the magnetization, phase transition and magnetocaloric effect from NdGaO₃.

4:25pm **PCSI-SuA-12 High-Efficiency Spin-to-Charge Conversion of Ultra-thin Mn₃Al/W Capping Layers on PLD Grown YIG**, *Manisha Dabla, Sanskriti Kaushik, Pushpendra Kumar*, Jawaharlal Nehru University, India; *Prashant Kumar*, Motilal Nehru College, India; *Bijoy K Kuanr*, Jawaharlal Nehru University, India

Ultra-Low-Power Spin-Orbit Torque (SOT) switching for next-generation Magnetic Random Access Memory (SOT-MRAM) is the result of high interfacial spin mixing conductance, which guarantees that any spin current generated in the heavy metal or through spin-momentum locking can seamlessly cross into the noncollinear antiferromagnet. This study investigates the enhancement of spin transport properties and magnetization dynamics in pulsed laser deposition (PLD) grown structures of GGG/YIG(20nm)[S-1], GGG/YIG(20nm)/Mn₃Al(2nm)[S-2] and GGG/YIG(20nm)/Mn₃Al(2nm)/W(5nm)[S-3]. Utilizing broadband ferromagnetic resonance (FMR), we evaluate the impact of the ultra-thin noncollinear antiferromagnet, Mn₃Al on YIG and the effect of heavy-metal Tungsten, W capping on spin pumping efficiency derived from Gilbert damping (a) from FMR linewidths (DH). The pure YIG film [S-1] exhibits an intrinsically low a (0.0015) for our PLD-grown films. Upon deposition of Mn₃Al(2nm) layer, a significant increase in the DH and hence enhanced effective damping a_{eff} (0.0027) are observed. This enhancement is attributed to the injection of a pure spin current from the precessing YIG layer into the Mn₃Al layer via spin pumping, which was confirmed by almost same zero-frequency DH₀ and AFM measured rms roughness. The spin transport efficiency is further amplified in the S-3 trilayer with enhanced a_{eff} (0.0041). The addition of the 5 nm W layer, known for its large spin Hall angle, acts as a highly efficient spin sink that maximizes the spin current gradient across the interfaces. Consequently, the calculated real part of the interfacial spin mixing conductance demonstrates a progressive and substantial enhancement from bilayer (5.9 × 10¹⁷ m⁻²) and trilayer

($1.25 \times 10^{18} \text{m}^{-2}$) configurations. These findings reveal that integrating W layers in addition to an ultra-thin Mn_3Al on the PLD-grown YIG significantly optimizes spin interfacial transparency, offering critical insights for the development of low-power, YIG-based spintronic/magnonic devices.

Figure 1 Caption Here

Figure 2 Caption Here

[1] I. Sinha, P. Kumar, A. Pandey, Bijoy K. Kuanr and S. Manna; Phys Rev. B **112**, 224428 (2025).

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edges and domain walls, that act as anharmonic confining potentials. This behavior is confirmed experimentally (Figure 1). We measure the expected nonlinear power-law scaling of amplitude, a systematic shift toward larger wavevector excitations at higher harmonic order, and a spin-selective response indicative of an increasingly chiral harmonic stray field. These results provide a microscopic understanding of magnonic harmonic generation and highlight its potential for engineering nonlinear functionality in magnonic systems.

[1] A. J. D'Addario, K. Hu, M. W. Olszewski, D. C. Ralph, M. E. Flatté, K. C. Nowack, and G. D. Fuchs, arXiv:2603.14082 (2026)

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4:30pm PCSI-SuA-13 Strain and Defect-Tailored Magnetotransport in Ferrimagnetic Spinel NiCo_2O_4 Thin Films and Freestanding Membranes,
Qiuchen Wu, Yuanyuan Zhang, Tianlin Li, Department of Physics and Astronomy & Nebraska Center for Materials & Nanoscience, University of Nebraska–Lincoln; **Myung-Geun Han,** Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory; **Soo-Yoon Hwang, Yeon-Seo Nam,** Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory; Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH); **Si-Young Choi,** Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Republic of Korea; **Yimei Zhu,** Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory; **Xia Hong,** Department of Physics and Astronomy & Nebraska Center for Materials & Nanoscience, University of Nebraska–Lincoln

The ferrimagnetic spinel NiCo_2O_4 (NCO) is a promising material for designing high-performance spintronic devices, while epitaxial strain and disorder can significantly modify its electronic and magnetic properties [1–3]. Here, we use epitaxial NCO thin films and freestanding NCO membranes as model systems to reveal the complex roles of strain and defects in determining its metallicity and magnetotransport [4]. Epitaxial 30 nm NCO films are deposited on spinel MgAl_2O_4 and perovskite SrTiO_3 and LaAlO_3 substrates. Freestanding NCO membranes are achieved by depositing 30 nm NCO film on $\text{Sr}_3\text{Al}_2\text{O}_6$ buffered LaAlO_3 followed by water etching. The NiCo_2O_4 films on MgAl_2O_4 show metallic behavior, small linear magnetoresistance (MR) with weak temperature dependence, and strong perpendicular magnetic anisotropy. In contrast, NCO on perovskite substrates and freestanding NCO membranes show insulating behaviors that can be well described by the contributions from thermal activation, nearest-neighbor hopping, and 3D variable range hopping. MR and anomalous Hall studies point to the existence of phase separation and spin canting in these samples, which is corroborated by electron microscopy studies. Comprehensive anisotropic magnetoresistance (AMR) studies show that NCO films on MgAl_2O_4 exhibit two-fold sinusoidal AMR, which can be well described by coherent rotation model. Additional four-fold AMR component emerges in the insulating samples, which can be attributed to disorder-induced spin scattering and strain-induced tetragonal magnetocrystalline anisotropy. It is noted that the NCO membrane exhibits highly consistent magnetotransport properties as the $\text{NiCo}_2\text{O}_4/\text{Sr}_3\text{Al}_2\text{O}_6$ film, showing that water etching does not alter the strain and disorder level in the system. Our study provides effective material strategies for engineering spin transport and magnetic anisotropy in NCO and presents a promising venue for designing flexible magnetic memory, sensor, and spintronic applications.

[1] Chen et. al., Adv. Mater. **31**, 1805260 (2019).

[2] Chen et. al., Appl. Phys. Lett. **120**, 242401 (2022).

[3] Xu et. al., J. Appl. Phys. **132**, 020901 (2022).

[4] Wu et. al., ACS Nano **20**, 11008 (2026).

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4:35pm PCSI-SuA-14 Imaging the Harmonic Generation of Magnons,
Gregory Fuchs, Cornell University **INVITED**

This work examines the mechanisms underlying the harmonic generation of magnons [1]. Harmonic generation is a nonlinear process that is well known in nonlinear optics, where a strong pump excitation frequency ω can generate tones at 2ω , 3ω , 4ω etc. I will describe our experiments imaging the harmonic generation of magnons in a $\text{Ni}_{81}\text{Fe}_{19}/\text{Pt}$ microstrip using a scanning nitrogen-vacancy (NV) center microscope. We analyze these measurements in a nonlinear spin-wave framework that is directly analogous to harmonic generation in nonlinear optics. Within this framework, the harmonic response arises from nonlinear magnetization dynamics localized at strongly inhomogeneous textures, such as the sample

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Room Ballroom - Session PCSI-SuE1

Plenary Session

Moderator: Christopher Palmström, University of California, Santa Barbara

7:30pm **PCSI-SuE1-1 Engineering Quantum Systems: From Qubits and Networks to Hybrid Quantum Matter**, *Tian Zhong*, University of Chicago

INVITED

The ability to control individual quantum systems - spins, photons, and solids - has enabled new approaches to computing, communication, and sensing. Extending this control from individual qubits to quantum matter calls for engineering both the microscopic constituents of a material and the electromagnetic fields through which they interact. In this talk, I will describe our efforts to develop quantum systems from the bottom up, beginning with long-coherence rare-earth qubit and quantum memories and progressing toward photonic control of nonequilibrium electronic states. The connecting theme is the co-design of materials and their optical environment, using thin-film growth and device integration to create quantum functionality.

Our approach begins with bottom-up rare-earth quantum materials grown by molecular-beam epitaxy. Telecom-wavelength erbium spin-photon interfaces combine long optical and spin coherence with compatibility with photonic and superconducting circuits, linking localized quantum degrees of freedom to photons that can propagate through optical fiber. I will discuss how epitaxial materials development and heterogeneous integration together provide a foundation for entangling spins to photons and, ultimately, optically interconnected quantum nodes. Building outward from these interfaces, we have also demonstrated a direct telecom quantum link between integrated entanglement source and erbium solid-state quantum memory, exploiting their intrinsic spectral matching without quantum frequency conversion.

We extend this approach to quantum matter by growing an ultrathin Bi_2Se_3 topological-insulator film directly on an on-chip silicon photonic-crystal cavity. This integration combines epitaxial growth and optical confinement while preserving access to time- and angle-resolved photoemission spectroscopy. Under resonant ultrafast excitation, we directly observe cavity-driven Floquet-Bloch sidebands with delayed buildup and a response prolonged beyond the incident pulse. The cavity thus controls both the spatial confinement and temporal evolution of the drive, establishing a platform for using engineered photonic environments to manipulate nonequilibrium electronic states.

These efforts share a common strategy: engineer quantum functionality from the material upward, and use innovations in heterogeneous integration to bring distinct quantum degrees of freedom into controlled interaction. I will conclude with an outlook on how co-designing materials and photonic structures may expand this range toward hybrid quantum interconnects and new forms of hybrid quantum matter.

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Room Ballroom - Session PCSI-SuE2

Quantum Networks & Rare-Earth Emitters

Moderator: Gregory Fuchs, Cornell University

8:15pm **PCSI-SuE2-10 Engineering Erbium-Doped Rare-Earth Oxide Thin Films For Quantum Networks**, *Jiefei Zhang*, Argonne National Laboratory

INVITED

Telecom spin qubits in semiconductors are of considerable interest for quantum memories and repeaters for quantum communication networks. Among the candidate systems, erbium ions (Er^{3+}) are especially promising because they provide a telecom C-band optical transition together with long-lived spin states, making them attractive for spin-photon interfaces. The development of CMOS-compatible erbium doped thin films is therefore an important step towards scalable Er^{3+} -based quantum devices. In this talk, we present a comparative study of two complementary approaches to this goal: (1) molecular beam epitaxy (MBE) of Er^{3+} doped oxide thin film on silicon [1-4] and (2) controlled spalling [5] of thin film from high-quality bulk Er^{3+} -doped crystal onto CMOS-compatible platforms. Specifically, we compare Er^{3+} doped CeO_2 thin film and spalled Er^{3+} doped CaWO_4 film to elucidate competing spin decoherence dynamics and the influence of surfaces/interfaces. The MBE grown Er^{3+} : CeO_2 exhibits a promising narrow optical homogeneous linewidth (~ 440 kHz) [2], a spin relaxation time of ~ 120 ms and a spin coherence of 38.8 μs at 77mK [3]. We identify spectral

diffusion driven by Er-Er spin flips as the dominant decoherence mechanism, with the large and symmetric g -tensor of this host playing a critical role in inducing strong Er-Er magnetic dipolar interactions. For comparison, we further explore an asymmetric host, CaWO_4 . By optimizing the spalling conditions for this medium-hard material, we obtain Er^{3+} : CaWO_4 films with thicknesses of ~ 1 microns. The spalled film shows a spin coherence of 347 μs , only 20% lower than that of bulk crystal (438 μs) [6]. In this host, the Er-Er interaction is governed by the much weaker $g \sim 1.2$ tensor component, significantly suppressing Er bath spin flip induced spectral diffusion. The modest reduction in coherence between spalled and bulk samples may be attributed to additional decoherence from dangling bonds and charges at the spalled surface. Finally, we discuss the trade-offs between epitaxial growth and crystal spalling as routes to scalable erbium-based quantum-network platforms, and outline mitigation strategies for reaching millisecond-scale spin coherence in integrated devices.

[1] G. Grant, et al. *APL Mater.* 12, 021121 (2024).

[2] J. Zhang, et al. *npj Quantum Information* 10,119 (2024)

[3] S. Seth, et al. *Phys. Rev. Lett.* 135, 266901 (2025)

[4] I. Masiulionis, et al. *APL Mater.* 13, 101116 (2025)

[5] C. P. Horn, et al., *ACS Nano* 18, 31381–31389 (2024).

[6] S. Seth, et al., manuscript under preparation

8:45pm **PCSI-SuE2-16 UPGRADED: A Fibre-Coupled Single-Erbium-Ion Source in Silicon Nanophotonics**, *Sven Rogge*, University of New South Wales, Australia

Erbium in silicon combines telecommunications C-band transitions with long optical and electron-spin coherence [1], but its millisecond lifetime constrains photon generation. Here, we demonstrate a fibre-coupled single-photon source from individual Er ions in silicon photonic-crystal cavities. Each device integrates 40 cavities (mode volume approximately $0.04 \mu\text{m}^3$; quality factor near 100,000) on a common bus waveguide, with approximately 50% measured waveguide-to-tapered-fibre outcoupling. Magnetic-field tuning brings individual Er transitions into resonance with the cavity modes. For the most strongly coupled ion, the excited-state lifetime is reduced from 1.68 ms to 1.5 μs , directly enhancing the total emission rate by more than a factor of 1000; correcting for the optical branching ratio implies a transition Purcell factor of approximately 5000. Pulsed Hanbury Brown and Twiss measurements give $g^2(0) = 0.001$, corresponding to a single-photon purity of approximately 0.999. A detected rate of approximately 3700 counts/s corresponds to an estimated in-fibre photon flux of approximately 60 kHz after accounting for excitation, spin shelving, optical transmission and detector efficiency. Similar lifetime reductions across cavities, and coupling of the same Er site in separate devices and fibre channels, demonstrate a reproducible fibre-addressed silicon architecture for telecom-band single-photon generation.

[1] I. R. Berkman et al., *npj Quantum Information* 11, 66 (2025).

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Room Ballroom - Session PCSI-MoM1

Superconducting & Hybrid Qubits

Moderator: Sue Coppersmith, University of New South Wales

8:30am PCSI-MoM1-1 Towards Scalable, Available, and Capable Superconducting Qubits, *Valla Fatemi*, Cornell University INVITED

In this seminar, I will present our team's recent efforts in developing high-performance superconducting qubits. Topics will include improving performance and processing windows of base layer films made from niobium and tantalum on silicon substrates, with special emphasis on the correlations between microwave quantum device performance and surface and interface materials properties [1,2]. Particularly, we found that we could reduce substrate temperatures for BCC Ta deposition well into the back-end-of-the-line process window via use of krypton as a sputtering gas. Transmon qubits with a twenty-micron capacitor gap made from these films exhibit quality factors exceeding fifteen million (coherence times up to 1 millisecond), demonstrating their performance with processing that is compatible with a greater number of tools. Additionally, I will highlight high-performance qubits made with Josephson junctions formed by a resist-free fabrication method [3] and our efforts to make high-performance qubit fabrication more broadly available through developing standard process flows at the Cornell Nanoscale Facility.

[1] Olszewski, Maciej W., Jadrien T. Paustian, Tathagata Banerjee, et al. "Low-Loss Nb on Si Superconducting Resonators from a Dual-Use Spintronics Deposition Chamber and with Acid-Free Post-Processing." *Applied Physics Letters* 128, no. 21 (2026): 214001. <https://doi.org/10.1063/5.0325435>.

[2] Olszewski, Maciej W., Lingda Kong, Simon Reinhardt, et al. "Krypton-Sputtered Tantalum Films for Scalable High-Performance Quantum Devices." arXiv:2601.20091. Preprint, arXiv, January 27, 2026. <https://doi.org/10.48550/arXiv.2601.20091>.

This prototype was primarily supported by the Microelectronics Commons Program, a DoW initiative, under award number N00164-23-9-G061. Funding (or Partial funding) for shared facilities used in this prototype was provided by the Microelectronics Commons Program, a DoW initiative, under award number N00164-23-9-G061.

[3] Banerjee, Tathagata, Stephen Daniel Funni, Saswata Roy, Judy J. Cha, and Valla Fatemi. "Resist-Free Shadow Deposition Using Silicon Trenches for Josephson Junctions in Superconducting Qubits." arXiv:2604.09796. Preprint, arXiv, April 10, 2026. <https://doi.org/10.48550/arXiv.2604.09796>.

9:00am PCSI-MoM1-7 Silicon Fin Based Josephson Junctions: Performance and Interfaces, *Roger Romani*, *Anthony McFadden*, NIST-Boulder; *Tenu van Schijndel*, UC Santa Barbara; *Trevyn Larson*, *Raymond Simmonds*, NIST-Boulder; *Chris Palmstrom*, UC Santa Barbara

Josephson Junctions (JJs) are a central building block of superconducting qubits and related technologies, but are known to host defects (so-called Two Level Systems, or TLS) which negatively impact the performance of quantum devices. Traditionally, JJs have been built around amorphous oxide barriers, which have long been thought to inherently host TLS. Here, we present a Josephson Junction based on a crystalline silicon fin, as proposed in the "FinMET" concept [1,2].

Our fin-based Josephson Junctions are fabricated using an anisotropic KOH etch on 110 Si using a SiN hard mask, creating fins approximately 1-2 μm tall and less than 20 nm thick. [3] Angle deposited aluminum forms electrodes on either side of the silicon fin, with the SiN forming a shadow mask that prevents shorting of the two electrodes over the top of the fin.

To test the performance of our fin-based JJs, we construct RF-SQUID style devices with the fin-based JJ acting as both a JJ and capacitor shunting a planar inductor. By measuring the resonant frequency of these structures as a function of the magnetic field threading the RF-SQUID loop, we see periodic modulation, unambiguous evidence that our fin-based element is acting as a Josephson Junction. Additionally, we search for and observe individual TLSs coupling to our device, inferring through their strong coupling that they are located within our fins. In future work, we aim to test whether these TLSs originate from defects in the aluminum-silicon interface or from the silicon fin itself, and develop methods for decreasing their density and impact on circuit performance.

9:05am PCSI-MoM1-8 Towards Single-Crystalline Tunnel Barriers on Epitaxial CoSi₂/Si for Low Loss Superconducting Circuits, *Julian Choi*, *Teun van Schijndel*, *Yu Wu*, *Chris Palmstrom*, UC Santa Barbara

Conventional Josephson junctions (JJs), superconductor/tunnel barrier/superconductor structures, are created using polycrystalline and amorphous materials. Typically, the superconducting metal layers are polycrystalline, and the tunnel barrier is amorphous, which leads to dangling bonds at the superconductor/tunnel barrier interfaces and in the tunnel barrier itself. These dangling bonds are believed to house two-level energy loss systems (TLS) that limit qubit and other quantum device performance.

Thus, one way to make progress in this field is to carefully select materials that minimize this loss. Cobalt disilicide (CoSi₂) can be grown epitaxially on silicon (Si), and its close lattice match with Si also enables the growth of single-crystalline Si tunnel barriers directly on the superconducting CoSi₂ layer [1, 2]. This prospect makes CoSi₂ particularly interesting for superconducting circuits because it eliminates the usage of amorphous or polycrystalline materials, which could potentially reduce loss. The vertical Josephson junction can then be completed by depositing another superconducting layer. In this talk, we demonstrate the growth and characterization of aluminum (Al)/Si/CoSi₂/Si(111) structures using molecular beam epitaxy. The reflection high-energy electron diffraction (RHEED) shows the signature 1x1 surface reconstruction for CoSi₂, 7x7 surface reconstruction post Si growth, and a 1x1 surface reconstruction following Al deposition. Following synthesis, atomic force microscopy of the CoSi₂ shows a smooth surface with terraces, which is indicative of a high-quality, epitaxial surface and suggests that the film grows in a well-ordered manner (Fig. 1 (a)). Additionally, the films exhibited sharp peaks in X-ray diffraction (Fig. 1 (b)) and oscillations in X-ray reflectivity, indicating well-defined crystalline structure and interfaces. Correlation of the growth parameters to the superconducting critical temperature of CoSi₂ were also investigated, with the highest critical temperature of 1.25 K.

[1]Ditchev, B. et al. *APL* **47**, 1200(1985), [2] Hensel, J. et al. *APL* **47**, 151 (1985)

9:10am PCSI-MoM1-9 UPGRADED: Cryogenic Deposition and Crystallization of Ultrathin Refractory Superconductors, *Teun van Schijndel*, *Yu Wu*, *Julian Choi*, *Milo Coombs*, *Jason Dong*, UC Santa Barbara; *Yilmaz Gul*, University College London, UK; *Greg Mazur*, *Christopher Palmstrom*, UC Santa Barbara

Refractory metals are important materials for superconducting electronics and quantum circuits. Many of these applications require thin films with controlled morphology and crystal structure, but achieving this control becomes particularly challenging at thicknesses of only a few nanometers. In conventional physical-vapor deposition, morphology and crystal structure depend strongly on adatom mobility, which is influenced by the substrate temperature relative to the melting temperature. Therefore, the high melting temperatures of refractory metals limit adatom mobility at typical substrate temperatures. However, increasing substrate temperatures can promote unwanted interfacial reactions, particularly with underlying III-V semiconductor heterostructures.

Here, we use cryogenic deposition to intentionally suppress atomic mobility and separate deposition from crystallization in ultrathin Nb, Ta, Re, and V films on III-V heterostructures. *In situ* reflection high-energy electron diffraction (RHEED) patterns show that Ta (Fig. 1(a)), Nb, and V films are initially highly disordered or amorphous and become polycrystalline upon heating to 250 °C (Fig. 1(b)). *Ex situ* Grazing-incidence X-ray diffraction (GIXRD) reveals that thinner Ta and Re films remain amorphous, whereas thicker films crystallize into α -Ta and hexagonal close-packed (hcp) Re (Fig. 1(c) and 1(d)). This thickness dependent behavior is confirmed for Re using scanning transmission electron microscopy (STEM) (Fig. 1(e) and 1(f)). In Ta/Nb bilayers, Ta crystallizes at a thickness of only 2 nm, indicating that adjacent metal layers can modify crystallization. Transport measurements reveal relationships between crystal structure and superconductivity. The α -Ta film shows a higher superconducting transition temperature (T_c) compared to amorphous Ta. In contrast, a 4 nm amorphous Re film has an enhanced T_c of 6.1 K, whereas 6 nm hcp Re has a T_c of 2.6 K. These results show how material choice, film thickness, and adjacent layers influence crystallization following cryogenic deposition, providing a pathway to integrate ultrathin refractory superconductors on III-V semiconductor heterostructures.

Monday Morning, January 18, 2027

9:25am **PCSI-MoM1-12 Quantum Oscillations in Semiconductor/Superconductor Hybrid Structures, *Greg Mazur*, University of California at Santa Barbara INVITED**

Hybrids of semiconductors and superconductors are the platform of choice for gateable and Andreev qubits and for quantum-dot Kitaev chains. However, the semiconductor parameters that enter the models of these devices are almost never measured in the hybrid itself. The superconductor shunts electrical transport, so density, mobility, effective mass and g-factor are inferred from etched Hall bars or uncapped sister wafers, which are physically different systems. Here we resolve this limitation by measuring the semiconductor directly beneath the superconductor through Shubnikov-de Haas (SdH) oscillations. In the disordered metal film the Landau levels are unresolved, so the oscillations originate from the semiconductor subbands alone, even when the film carries most of the current. We study a 7-nm InAs quantum well beneath a 10-nm $\text{In}_{0.75}\text{Ga}_{0.25}\text{As}$ barrier, capped at 7 K with Al, Sn, V, Nb, Ta or Re films, and introduce a Dingle analysis that accounts for the shunt and returns quantum lifetimes that are stable across analysis temperatures. Remarkably, every metal adds an interface subband that is absent from the bare well. Its density falls into two classes that do not follow the work function, $(5.3-6.5) \times 10^{11} \text{ cm}^{-2}$ beneath the d-band metals V, Nb, Ta and Re and $(1.2-1.3) \times 10^{12} \text{ cm}^{-2}$ beneath Al and Sn, pointing to Fermi-level pinning at two distinct levels. A Re thickness series places this state within a few nanometres of the metal, while the well 10 nm below is unaffected. Importantly, the buried well retains its properties beneath all six films: its cyclotron mass $(0.040-0.044 m_e)$ and $|g| = 4.9 \pm 0.2$, extracted from spin zeros in tilted field, match the uncapped well, and no film shortens its quantum lifetime, while Al and Sn lengthen it. The lifetimes bound the hybridization of the interface subband to 2-4 meV. Crucially, these are the normal-state parameters that tunnelling spectroscopy renormalizes but cannot access. Combined, the two techniques pin down the materials parameters of hybrid devices, and quantum oscillations emerge as a general tool to characterize the semiconductor in the stack in which it is actually used, on any platform in which the oscillations survive metallization.

9:55am **PCSI-MoM1-18 Predicting the Structure and Properties of Inorganic Epitaxial Interfaces, *Noa Marom*, Carnegie Mellon University INVITED**

Epitaxial inorganic interfaces lie at the heart of semiconductor, spintronic, and quantum devices. At an interface between two dissimilar materials physical properties and functionalities may arise, which do not exist in any of the isolated constituents in the bulk. The resulting device performance hinges on the electronic and magnetic properties of the interface. The configuration space of possible inorganic interfaces is vast and largely underexplored, owing to the almost infinite number of ways different materials can be combined to form interfaces. Computer simulations may significantly accelerate the discovery and design of new inorganic interfaces with desirable properties.

To predict the structure of domain-matched epitaxial interfaces, we have developed the OGRE code [1]. OGRE starts by performing “lattice matching” to identify all possible domain-matched commensurate interfaces within the range of user-defined Miller indices, maximum strain, and maximum area. For each orientation, OGRE constructs interface structures by identifying and combining all possible surface terminations of the two materials. Subsequently, for each interface, OGRE performs “surface matching” to identify the best in-plane registry and interfacial distance between the two materials. Finally, all candidate interfaces are ranked by stability.

To study the electronic properties of interfaces we use density functional theory (DFT). Within DFT, the many-body interactions between electrons are described by approximate exchange-correlation functionals. The accuracy of the results hinges on an appropriate choice of functional. We have developed a method of machine learning the Hubbard U correction added to a DFT functional by Bayesian optimization (BO) [2]. The DFT+U(BO) method balances accuracy with computational cost, enabling unprecedented simulations of large surface and interface models of interest for applications in quantum computing. For example, we have used DFT+U(BO) to assess candidate materials for tunnel barriers at semiconductor/ superconductor interfaces [3,4].

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[2] M. Yu, S. Yang, C. Wu, and N. Marom, npj Computational Materials 6, 180 (2020)

[3] M. J. A. Jardine, D. Dardzinski, M. Yu, A. Purkayastha, A.-H. Chen, Y.-H. Chang, A. Engel, V. N. Strocov, M. Hocevar, C. J. Palmström, S. M. Frolov, and N. Marom, ACS Applied Materials & Interfaces 15, 16288 (2023)

[4] M. J. A. Jardine, D. Dardzinski, Z. Cai, V. N. Strocov, M. Hocevar, C. J. Palmström, S. M. Frolov, and N. Marom, ACS Applied Materials & Interfaces 17, 5462 (2025)

PCSI

Room Ballroom - Session PCSI-MoM2

Point Defects & Quantum Emitters

Moderator: Sven Rogge, University of New South Wales, Australia

11:00am **PCSI-MoM2-31 Next-Generation Integrated Quantum Technologies with Thin-Film, Single-Crystal Diamond, *Alex High*, University of Chicago INVITED**

Diamond is the leading solid-state platform for quantum networking and room-temperature deployable quantum sensing technologies. The continued evolution of quantum technologies in diamond requires heterogeneous material platforms for sophisticated functionalities, device integration and packaging, and improved qubit performance. At UChicago and Argonne National Laboratory, we are creating pristine single-crystal diamond thin-films that host coherent color center qubits and utilizing direct-bonding processes to integrate them with a wide range of materials including fused silica, sapphire, thermal oxide, lithium niobate, tantalum, silicon and YIG (figure 1).¹ High-resolution imaging of a diamond membrane/sapphire interface showcases crystalline reconstruction, signifying bonding between the diamond and host substrate, and hosted color centers maintain excellent coherence throughout processing (figure 2).

In this talk, I will present our diamond thin-film synthesis and integration methods, and present in-depth characterization of the thin-films following integration, and update on recent results from the Advanced Photon Source at Argonne. I will highlight performance of the thin-films in quantum device architectures for networking and sensing, including record-setting qubit and photonic performance. I will demonstrate how material heterostructures composed of thin-film diamond bonded to thin-film lithium niobate unlock new functionalities for quantum networking nodes. For instance, we show that by utilizing the piezoelectric effect in lithium niobate, we can dynamically control strain within the diamond layer and tune critical qubit properties. I will also demonstrate how integration of thin-film diamond with glass substrates can be utilized to generate significant tensile strain in diamond, unlocking axial-free qubits within the diamond.

11:30am **PCSI-MoM2-37 UPGRADED: Atomic Defects and Quantum Light Sources in van der Waals $\alpha\text{-MoO}_3$, *Jeonghan Lee*, Seoul National University, Republic of Korea; *Haiyuan Wang*, Technical University of Denmark; *Keun-Yeol Park*, Soonsang Huh, Donghan Kim, Mihyang Yu, Changyoung Kim, Seoul National University, Republic of Korea; *Kristian Thygesen*, Technical University of Denmark; *Jieun Lee*, Seoul National University, Republic of Korea**

Atomic defects in solid-state materials have attracted much recent attention due to their potential to realize photonic quantum information processing in various material platforms. Quantum light sources from atomic defects in two-dimensional (2D) materials have been particularly promising for developing quantum technologies in van der Waals (vdW) materials and heterostructures. However, studies on room-temperature (RT) quantum emitters in 2D materials have been limited so far, urging the identification of novel 2D materials that can host RT quantum emitters to enable a wider range of fundamental studies and quantum applications. In this talk, we present the observation of RT quantum emission from $\alpha\text{-MoO}_3$, a vdW semiconductor which has a bandgap of 3 eV [1]. By annealing exfoliated ultrathin $\alpha\text{-MoO}_3$ flakes, we found localized sharp emitter peaks around the energy of 2 eV. With the photon antibunching curve in the second-order correlation function measurements, single-photon nature of the emitted light is demonstrated. The density functional theory calculation further supports that the oxygen vacancy center is a highly promising candidate of the observed emitters. Our work provides $\alpha\text{-MoO}_3$ as a novel platform to study atomic defects and quantum light sources in vdW systems for realizing RT quantum technologies.

[1] J. Lee, H. Wang, K.-Y. Park, S. Huh, D. Kim, M. Yu, C. Kim, K. S. Thygesen, J. Lee, Nano Lett. 25, 1142 (2025).

11:45am **PCSI-MoM2-40 UPGRADED: Transition from Single-Photon Emission to Superradiance in Dense WSe₂ Quantum Emitter Arrays**, *Frances Camille Wu*, The University of Texas at Austin; *Shang-Hsuan Wu*, *Jadon Zheng*, *Kenneth Lin*, University of Texas at Austin; *Bin Fang*, The University of Texas at Austin; *Suhun Kim*, *Emanuel Tutuc*, *Edward Yu*, University of Texas at Austin

Cooperative light emission arises when multiple indistinguishable quantum emitters interact coherently through a shared electromagnetic field, dramatically changing emission characteristics and offering opportunities for generating entangled quantum states for quantum computing, quantum information processing, and secure communications. A key example is superradiance, in which coupled quantum light emitters radiate collectively and emit in phase, producing an enhanced, high-intensity burst of light.¹ However, superradiance remains challenging to realize in solid-state materials because it requires interacting emitters to be identical, while quantum emitters in these systems are inevitably subject to variations in their local environment, including strain, carrier fluctuations, and surrounding defects. Two-dimensional semiconductors, particularly monolayer tungsten diselenide (WSe₂), offer a promising platform due to their atomically thin structure, strong excitonic interactions, and sensitivity to local strain, enabling spatial and spectral control of quantum emitters which provides new opportunities for realizing scalable cooperative quantum light sources.

In this work, we demonstrate superradiant emission and the transition from single-photon to superradiant light emission in strained monolayer WSe₂ suspended over dense nanocavity arrays, with uniform localized strain controlled through electrostatic interactions.² Computational studies have predicted a critical inter-emitter spacing for achieving superradiance in two-dimensional systems, where is the emission wavelength.³ By comparing devices with inter-emitter spacings of and , we show that emitters remain isolated single-photon sources when , whereas reducing the spacing below this threshold produces pronounced photon bunching, fast radiative lifetime, and enhanced peak intensity—the characteristic signatures of superradiance. Furthermore, electrostatic back-gating enhances both emitter intensity and superradiant emission, consistent with increased exciton populations funneling toward deeply bound defects under electrostatic gating. These results demonstrate a powerful new platform for highly controlled, large-scale quantum light emission in two-dimensional materials, and establish inter-emitter spacing and electrostatic gating as effective controls for engineering cooperative quantum light emission in two-dimensional materials.

12:00pm **PCSI-MoM2-43 Nitrogen-Vacancy-Related States in Ga- and N-Polar GaN by XPS and First-Principles Calculations**, *Chisato Ota*, *Tomoe Yayama*, *Takeyoshi Onuma*, *Tomohiro Yamaguchi*, Kogakuin University, Japan; *Masatomo Sumiya*, NIMS (National Institute for Materials Science), Japan; *Tohru Honda*, Kogakuin University, Japan

N-polar InGa_{0.5}Ga_{0.5}N/GaN heterostructures are attractive for optoelectronic and energy-conversion devices because the reversed polarization field can facilitate the separation and extraction of photogenerated carriers. However, point defects may limit their optical and electronic properties through nonradiative recombination. The photothermal deflection spectroscopy signal intensity in the bandgap was higher for N-polar GaN than for Ga-polar GaN, suggesting a larger contribution from defect-related states. In this context, experimental characterization of nitrogen vacancies (V_N) remains a crucial issue. We investigated the valence-band states of Ga- and N-polar GaN by X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations. The measured spectra were compared with calculated densities of states (DOS) for pristine GaN and GaN containing V_N. The pristine GaN DOS reproduced the Ga-polar spectrum well, whereas the N-polar sample showed a tail-like feature near the valence-band maximum that was not reproduced by the pristine calculation. Calculations including V_N produced additional states in the corresponding energy region. To evaluate V_N, the difference DOS, DOS_{VN} - DOS_{pristine}, was compared with the residual XPS spectrum obtained by subtracting the scaled defect-free DFT spectrum from the experimental XPS spectrum. The broadened difference DOS was scaled to reproduce the experimental residual spectrum. From the scaling factor, the near-surface V_N concentration in the N-polar sample was estimated to be approximately 6 × 10¹⁹ cm⁻³. These results suggest that valence-band XPS combined with first-principles calculations can provide an approach for evaluating V_N-related electronic states in GaN.

PCSI

Room Ballroom - Session PCSI-MoA1

Superconductivity in Thin Films & Heterostructures

Moderator: Monica Allen, University of California at San Diego

2:00pm **PCSI-MoA1-1 Thin Film Quantum Matter: Unconventional Conventional Superconductivity and More, Joseph Falson**, California Institute of Technology **INVITED**

In this presentation I will discuss recent intermetallic and oxide thin film materials we have grown in our lab, including an array of ultra-thin materials which display magnetic field-induced superconductivity, along with topological materials which are sufficiently clean to show the quantum Hall effect. I will take time to emphasize the correlations between the unique synthesis pathways these compounds take and the physics they display, with the goal of connecting an understanding of subtle physical and chemical distortions with the ability to resolve profound emergent electronic phases.

2:30pm **PCSI-MoA1-7 Stoichiometric FeTe is a Superconductor, Cui-Zu Chang**, The Pennsylvania State University **INVITED**

In this talk, I will first briefly introduce the molecular beam epitaxy (MBE) growth mechanism, and then focus on our recent progress in the MBE growth of FeTe films and heterostructures. FeTe, unlike its superconducting isostructural counterpart FeSe, has long been regarded as an antiferromagnetic (AFM) metal sans superconductivity. Over the past five years, my group has employed MBE to synthesize a series of FeTe-based heterostructures, in which superconductivity consistently emerges. More recently, we developed an approach to grow FeTe thin films followed by post-growth annealing under a Te flux. Using spin-polarized scanning tunneling microscopy and spectroscopy (STM/S), we show that the AFM order in as-grown FeTe films originates from interstitial Fe atoms that disrupt the ideal 1:1 stoichiometry. Remarkably, removing these interstitial Fe atoms via Te annealing produces stoichiometric FeTe films that exhibit no AFM order and instead display robust superconductivity with a critical temperature of ~ 13.5 K. This superconducting state is further confirmed by the observation of Cooper-pair tunneling, zero electrical resistance, and the Meissner effect. Based on these results, we establish a new phase diagram for Fe_{1-x}Te and demonstrate that stoichiometric FeTe is inherently a superconductor, overturning a long-held view that it is an AFM metal [1]. Building on the superconducting stoichiometric FeTe films, we further used MBE to grow a one-quintuple-layer trigonal $(\text{Bi,Sb})_2\text{Te}_3$ layer on top of six-unit-cell tetragonal FeTe. We realized moiré engineering of Cooper-pair density modulation (CPDM) states and demonstrated that CPDM states are a universal phenomenon in moiré superconductors [2].

[1] Yan et al., *Nature* **652**, 342–348 (2026).

[2] Wang et al., *Nature* **652**, 335–341 (2026).

3:00pm **PCSI-MoA1-13 Robust Superconductivity against Al Substitution in LiTi_2O_4 Thin Films, Elijah Robinson, Kashi Panday, Gabe Manzanera, Prakash Timsina, Sudhan Koirala, Stefan Zollner, Igor Vasiliev, Ludi Miao**, New Mexico State University

The origin of superconductivity in LiTi_2O_4 remains an important question because its mixed-valence Ti network supports a complex electronic state in which carrier filling, disorder, and charge frustration may influence pairing. Building on earlier substitution studies [1], we grow Al-substituted $\text{Li}(\text{Ti}_{1-x}\text{Al}_x)_2\text{O}_4$ thin films on $\text{MgAl}_2\text{O}_4(001)$ by pulsed-laser deposition to test how superconductivity responds when this network is chemically perturbed. Superconductivity persists up to nominal 50% Ti-site substitution even as the normal state becomes substantially more resistive (Fig. 1). This contrast indicates that normal-state conduction and superconductivity have markedly different sensitivities to Al substitution. Zero-resistance transitions and comparatively stable transition temperatures and upper-critical-field scales support the robustness of superconducting transport. The fourfold angular response previously reported in undoped films [2] also survives at the heavily substituted endpoint. Structural characterization reveals lattice contraction, while spectroscopic ellipsometry and density-functional calculations probe the accompanying electronic evolution. The calculations identify stoichiometric LiTiAlO_4 as a carrier-depleted limit, emphasizing that Al substitution changes nominal electron filling and Ti connectivity as well as introducing nonmagnetic disorder. The superconducting response must therefore be understood in the context of a changing electronic system, beyond a simple impurity-scattering picture. Because Al substitution is expected to disrupt the mixed-valence network that can support charge frustration, persistent

superconductivity argues against charge frustration on an intact Ti network being essential to pairing. These films provide a platform for disentangling the roles of carrier filling, disorder, and charge frustration in oxide superconductivity.

[1] P. M. Lambert, P. P. Edwards, and M. R. Harrison, *J. Solid State Chem.* **89**, 345–360 (1990).

[2] H. Xue et al., *ACS Nano* **16**, 19464–19471 (2022).

3:05pm **PCSI-MoA1-14 Characterization of Thin Films for Quantum Information Science, Jesus Marquez**, New Mexico State University

Thin films play a vital role in the development of technologies such as spintronics, low-power-loss electronics, and quantum computing. We characterized thin films to study their unique properties, such as aluminum (Al) and bismuth antimony (BiSb) thin films. BiSb thin films have been characterized using scanning tunneling microscopy (STM); images show nanoscale structures such as triangles, bright interconnected loops, steps, and smooth surfaces, indicating a high-quality film, similar to Bi thin films [1]. Al thin films capped with silicon have been characterized using the physical properties measurement system (PPMS) to measure the critical temperature (T_c) of superconductivity, and results indicate an enhancement of superconductivity compared to the T_c of bulk aluminum, similar to uncapped Al thin films [2]. Properties of BiSb and Al thin films have been obtained using techniques such as STM and PPMS; characterizing thin films is important to study their effects and harness their properties for potential future technologies. This work is supported by NSF DMR 233941 and NSF PREM grant DMR-2423992.

[1] Dong, J. T., Inbar, H. S.; Dempsey, C. P., Engel, A. N., Palmstørn, C. J. Strain Solitons in an Epitaxially Strained van der Waals-like Material. *Nano Lett.* (2024) **24** (15): 4493–4497.

[2] van Weerdenburg, W. M. J.; Kamlapure, A.; Fyhn, E. H.; Huang, X.; van Mullekom, N. P. E.; Steinbrecher, M.; Krogstrup, P.; Linder, J.; Khajetoorians, A. A. Extreme enhancement of superconductivity in epitaxial aluminum near the monolayer limit. *Science Advances*. (2023)

3:10pm **PCSI-MoA1-15 Interplay of Ferromagnetism and Superconductivity in Fe-Doped Ferromagnetic Semiconductors, Anh Le Duc, Hirotaka Hara**, The university of Tokyo, Japan; **Masaaki Tanaka**, The University of Tokyo, Japan **INVITED**

The interplay between superconductivity and ferromagnetism gives rise to unconventional phenomena, including Josephson π -junctions, spin-triplet pairing, and superconducting diode effects, and offers opportunities for exploring Majorana physics. Fe-doped narrow-gap III–V ferromagnetic semiconductors (FMSs) provide a distinctive platform for investigating this interplay by combining ferromagnetic exchange coupling with semiconductor functionality and electrical tunability. Unlike conventional ferromagnetic Josephson junctions, their carrier density and magnetic interactions can be controlled through electrostatic modulation. Our earlier Nb/(In,Fe)As Josephson junctions exhibited long-range proximity-induced superconductivity and unusual magnetic interference patterns, providing evidence for spin-triplet electron pairing [1].

Here, we present two recent advances in epitaxial superconductor/FMS heterostructures grown in situ by molecular beam epitaxy. First, Al films deposited directly on strained (In,Fe)As exhibit superconductivity below 1.1–1.4 K [2]. The dominant Al growth orientation changes from (110) to (111) with increasing the in-plane lattice constant of (In,Fe)As, while superconducting properties correlate with Al morphology and grain size. An anomalous decrease in the critical magnetic field below 0.5 K suggests possible magnetic coupling across the Al/(In,Fe)As interface.

Second, Al/InAs/(Ga,Fe)Sb heterostructures integrate superconducting and magnetic proximity effects in an InAs channel with atomically sharp interfaces [3]. Electrostatic gating can modulate the carrier density in InAs and its wavefunction overlap with the adjacent FMS(Ga,Fe)Sb, offering a route to controlling both Josephson coupling and magnetic proximity interactions. The fabricated junctions exhibit gate-tunable supercurrents and multiple Andreev reflections up to sixth order. Hysteretic and asymmetric Fraunhofer interference patterns provide evidence of induced ferromagnetism and broken time-reversal symmetry. Nonreciprocal critical currents demonstrate a superconducting diode effect with efficiency reaching 20%, while interference analysis suggests enhanced supercurrent near the channel edges. These results establish a promising platform for electrically tunable superconducting spintronics and motivate further exploration of unconventional pairing, topological superconductivity, and Majorana modes.

[1] T. Nakamura, L. D. Anh, Y. Hashimoto, S. Ohya, M. Tanaka, and S. Katsumoto, Phys. Rev. Lett. 122, 107001 (2019).

[2] H. Hara et al., APL Materials (2026, in press); arXiv:2609.04744.

[3] H. Hara, L. Baker et al., Communications Materials (2026, in press); arXiv:2603.17101.

PCSI

Room Ballroom - Session PCSI-MoA2

Oxides I

Moderator: Jiefei Zhang, Argonne National Laboratory

4:30pm **PCSI-MoA2-31 Ferroelectric-Control of Magnetotransport in Ruddlesden-Popper Strontium Iridates, Xia Hong**, University of Nebraska-Lincoln **INVITED**

The Ruddlesden-Popper $5d$ iridates $Sr_{n+1}Ir_nO_{3n+1}$ (SIO) represents a model system where the close competition between charge itinerancy, strong spin-orbit coupling, and onsite Coulomb energy can lead to a rich phase diagram. Nonvolatile voltage control of their electronic and magnetic properties is of intensive research interests for designing emergent quantum states and developing novel energy-efficient device applications, which is yet to be demonstrated. This talk discusses the tuning of magnetotransport properties of ultrathin SIO ($n = 1, 2, \infty$) films via interfacial ferroelectric $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) (Fig. 1a). Nonvolatile polarization control of metal-insulator transition (MIT) has been achieved in $SrIrO_3$ and $Sr_3Ir_2O_7$. Bulk $SrIrO_3$ is a correlated semimetal. In the 2D limit, $SrIrO_3$ thin films exhibit weak (anti)localization [1], which are modulated via PZT polarization reversal. Anomalous Hall and topological Hall effects are observed in PZT/ $SrIrO_3$ close to the MIT, signaling emergent magnetism. All-oxide ferroelectric tunnel junctions (FTJs) composed of $LaNiO_3$ (LNO)/PZT/ $Sr_3Ir_2O_7$ exhibit significantly enhanced electroresistance (ER) at room temperature (RT) compared with FTJs exploiting other correlated oxide electrodes (Fig. 1b), which can be attributed to polarization induced MIT in interfacial $Sr_3Ir_2O_7$ [2]. While single-layer Sr_2IrO_4 is a $J=1/2$ Mott insulator, the PZT/ Sr_2IrO_4 heterostructure shows transport characteristic of a 2D correlated metal (Fig. 1c) due to the interfacial charge transfer effect [3]. The in-plane magnetoresistance (MR) and out-of-plane anisotropic MR show distinct temperature and magnetic field dependences for single-layer Sr_2IrO_4 and PZT/ Sr_2IrO_4 (Fig. 1d), suggesting polarization controlled magnetic anisotropy and possible emergence of incipient ferromagnetism. These results showcase how charge-, lattice-, and symmetry-mediated interfacial coupling with ferroelectrics can be leveraged to induce emergent phenomena and design voltage-controlled functionalities in $5d$ iridates.

[1] L. Zhang et al, APL Materials **8**, 051108 (2020).

[2] Y. Zhang et al, Applied Physics Letters **125**, 102904 (2024).

[3] Y. Zhang et al, Advanced Physics Research **4**, 2400208 (2025).

5:00pm **PCSI-MoA2-37 UPGRADED: Observation of Field-Induced Interface Reactions in HfO_2 -Based Ferroelectric Devices by HAXPES, Takashi Onaya, Takahiro Nagata, Kazuhito Tsukagoshi, Toshihide Nabatame**, National Institute for Materials Science, Japan

Ferroelectric HfO_2 -based materials are attractive for future nonvolatile memory devices due to their excellent CMOS compatibility and thickness scalability (<10 nm) [1]. However, it remains critical reliability issues in practical applications such as fatigue and hard breakdown during electric field cycling [2]. These endurance degradations were thought to be mainly caused by the formation of defects such as oxygen vacancies (V_O) in HfO_2 -based films [3], but it has been unclear why V_O increases during field cycling. In this study, we investigated the interface reaction between the ferroelectric $Hf_{x}Zr_{1-x}O_2$ (HZO) film and TiN electrode during field cycling by synchrotron hard X-ray photoelectron spectroscopy (HAXPES) to clarify the origin of endurance degradation.

Three different switching cycles, such as pristine for 10^0 , wake-up for 10^4 , and fatigue for 10^8 , were applied to TiN/HZO (10 nm)/TiN ferroelectric capacitors. Then, chemical states of Ti at the HZO/TiN bottom-electrode interface were evaluated by synchrotron HAXPES with the X-ray energy of 8 keV after removal of TiN top-electrodes. In the pristine state, Ti-O (~ 4969 eV) and Ti-N peaks (~ 4966 eV) of Ti 1s spectra were observed, indicating that a TiO_xN_y interfacial-layer (IL) was formed at the HZO/TiN interface. In the wake-up state, no difference of Ti 1s spectra was observed between the pristine and wake-up states. Therefore, the HZO/TiN interface did not change during wake-up field cycling. In the fatigue state, on the other hand, the Ti-O and TiO_xN_y components increased compared to those of the

pristine and wake-up states. This indicates that an oxygen-rich and thicker TiO_xN_y -IL formed at the HZO/TiN interface. Therefore, a field-induced interface reaction accompanied by oxygen diffusion from the HZO film to TiN electrodes should occur during fatigue field cycling, resulting in additional V_O formation in the HZO film. In conclusion, we clarified one of the origins of endurance degradation by evaluating field-induced interface reactions using synchrotron HAXPES.

[1] T. S. Böske et al., Appl. Phys. Lett. **99**, 102903 (2011).

[2] M. Pešić et al., Adv. Funct. Mater. **26**, 4601 (2016).

[3] W. Hamouda et al., Appl. Phys. Lett. **120**, 202902 (2022).

5:15pm **PCSI-MoA2-40 Ferroelectric Control of Metallicity and Magnetism in Ultrathin Sr_2IrO_4 Films, Yuanyuan Zhang, Qiuchen Wu, Yifei Hao, Peace Adegbite, Peter Dowben, Xia Hong**, University of Nebraska-Lincoln

The Ruddlesden-Popper $5d$ iridate Sr_2IrO_4 is an antiferromagnetic Mott insulator in which the electronic, magnetic, and structural states are strongly coupled. Achieving nonvolatile voltage control of its electronic and magnetic properties is of significant fundamental and technological interests. Here, we report the ferroelectric control of metallicity and magnetism in ultrathin Sr_2IrO_4 via interfacial ferroelectric $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) [1]. Reversing the polarization of PZT induces nonvolatile, reversible resistance modulation in Sr_2IrO_4 . The conductance of PZT/ Sr_2IrO_4 in both polarization states is predominantly above the quantum conductance of e^2/h and exhibits $\ln(T)$ behavior, which is characteristic of a 2D weakly localized metal. This behavior is in sharp contrast to the 3D variable range hopping (VRH) behavior observed in single-layer Sr_2IrO_4 , suggesting that interfacing with PZT induces a metal-insulator transition and dimensionality crossover. X-ray photoelectron spectroscopy reveals significant charge transfer at the interface, corroborated by Hall effect measurements, which can account for the enhanced metallicity.

In the single-layer sample, the in-plane MR exhibits low-field hysteresis associated with the antiferromagnetic spin-flip transition below 160 K, together with a large negative MR. In contrast, the heterostructure shows negligible low-field hysteresis with positive MR dominating down to 6 K. Below 6 K, the MR exhibits an opposite field-dependence compared with the single-layer sample, i.e., positive MR at low field followed by negative MR at high field, with a magnitude one order smaller. In addition, field-sweep-rate-dependent resistance dip is observed in the heterostructure, possibly associated with an incipient ferromagnetic state.

Switching the polarization of PZT modulates the out-of-plane anisotropic magnetoresistance R_{AMR} . For the polarization up state, unusual multi-level resistance pinning appears in R_{AMR} below 30 K, indicating polarization modulation of magnetic anisotropy. These results reveal the charge-mediated emergent phenomena at the ferroelectric/ Sr_2IrO_4 heterointerface.

[1] Y. Zhang, Q. Wu, Y. Hao, et al., Adv. Phys. Res. **4**, 2400208 (2025).

PCSI

Room Ballroom - Session PCSI-MoE

High-k Dielectrics & Devices Interfaces

Moderator: Xia Hong, University of Nebraska - Lincoln

7:30pm PCSI-MoE-1 UPGRADED: Time Evolution of Surface Chemical Reactions During Aluminum Oxide Atomic Layer Deposition on InAs, Rainer Timm, **Eleni Charitoudi**, Nishant Patel, Lund University, Sweden; Rosemary Jones, Esko Kokkonen, Max IV Laboratory, Sweden

III-V semiconductors have highly promising properties for electronic applications. Specifically, InAs has a narrow, direct band gap and high electron mobility, making it a good candidate to outperform Si-based Metal Oxide Semiconductor Field-Effect Transistors (MOSFETs) in terms of speed and power consumption. The detrimental native oxide should thereby be replaced by a so-called high-k oxide, such as Al_2O_3 , improving the gate properties. However, the performance of this system is limited by a high defect density at the InAs/ Al_2O_3 interface,¹ which is attributed to the incomplete removal of the native oxide layer.

The precise deposition of Al_2O_3 on InAs is achieved via atomic layer deposition (ALD), enabling the production of thin films with atomic-scale precision. It is characterised by a layer-by-layer mechanism and the self-limiting interaction between two gaseous precursors and the substrate. In our case, two half-cycle depositions were performed using trimethylaluminum (TMA) and water as precursors. A common method for studying the chemical composition and interface quality of ALD films is to perform X-ray photoelectron spectroscopy (XPS) measurements before and after each half-cycle. Here, we instead use ambient-pressure XPS (AP-XPS) to monitor time-resolved surface chemical reactions during ALD half-cycles in the implemented ALD cell at the SPECIES synchrotron beamline of the MAX IV Laboratory.²

Upon ALD, the As-oxide was found to get entirely removed during the initial TMA half-cycle (TMA), as shown in **Figure 1** (supplemental document). This self-cleaning is far less efficient for the In-oxide, which only decreases slightly in intensity. More interestingly, the type of In-suboxide changes upon ALD, resulting in a decreased In oxidation state after TMA deposition and an increased oxidation state after water pulsing. Such a re-oxidation of the substrate material upon ALD, in parallel with the wanted formation of Al_2O_3 , is unexpected, and it is in contrast with previous results from AP-XPS measurements of HfO_2 ALD on InAs.^{3,4} Here, we will compare the two high-k ALD processes based on reaction dynamics observed from time-resolved In, As, Al, Hf, and C core-level spectra, including different organic ligands and reaction byproducts.

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4. D'Acunto, G. et al., Surfaces and Interfaces 39, 102927 (2023)

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7:45pm PCSI-MoE-4 Direct Evaluation of $\text{SiO}_2/\text{Al}_2\text{O}_3$ Interface Dipole for Si/ $\text{SiO}_2/\text{Al}_2\text{O}_3/\text{HfO}_2$ Gate Stack Using Operando HAXPES, Masaki Ando, Meiji University, Japan; Takashi Onaya, Toshihide Nabatame, National Institute for Materials Science (NIMS), Japan; Satoshi Toyoda, Office of Institutional Advancement and Communications, Kyoto University, Japan; Atsushi Ogura, Meiji University, Japan

Background: Dipole techniques have been investigated to control the threshold voltage (V_t) in n- and p-FETs, and Al_2O_3 has been proposed as a candidate dipole material for p-FETs [1,2]. An Al_2O_3 dipole layer is inserted at the $\text{SiO}_2/\text{HfO}_2$ interface of Si/ $\text{SiO}_2/\text{HfO}_2$ gate stacks, and its thickness is controlled by the number of atomic layer deposition (ALD) cycles. V_t is known to be affected by both fixed charges and dipoles in the gate stack; however, it has been difficult to separate them by electrical measurements. In this study, we directly evaluate the $\text{SiO}_2/\text{Al}_2\text{O}_3$ interface dipole in Si/ $\text{SiO}_2/\text{Al}_2\text{O}_3/\text{HfO}_2$ stacks using hard X-ray photoelectron spectroscopy under gate bias (operando HAXPES) [3].

Experiment: Al/p-Si/ SiO_2 (9 nm)/ Al_2O_3 (0 or 0.2 nm)/ HfO_2 (4 nm)/Pt stacks were prepared using ALD. Using operando HAXPES at SPring-8 BL46XU ($h\nu = 7.94$ keV, $|V_g| \leq 1.5$ V), Hf 3d, Si 1s and Pt 3d spectra were acquired while applying a gate voltage [Fig. 1(a)]. As each core level follows its layer's potential, $\text{sep}_c = \text{BE}(\text{Si } 1s (\text{Si}^{4+})) - \text{BE}(\text{Hf } 3d_{5/2})$ gives the $\text{HfO}_2\text{-SiO}_2$ potential difference across Al_2O_3 . The measured interface dipole was corrected as

sep_c reflects only 60% of the actual value due to a 40% V_g drop between Hf 3d and Si^{4+} .

Results: The Al_2O_3 -induced change in sep_c was 0.14 ± 0.03 eV after correction for the V_g drop [Fig. 1(b)]. This actual interface dipole was independent of V_g and polarity [Fig. 1(b),(c)], excluding the possible influence of mobile ions and charge trapping. The sep_c of the 0.4-nm-thick Al_2O_3 sample was almost the same due to saturation of the dipole effect (data not shown). Both the corrected sep_c value and saturation trend are consistent with reported C-V results (V_b shift of +0.14 to +0.25 V) [4]. Thus, operando HAXPES is a promising analysis method to evaluate the $\text{SiO}_2/\text{Al}_2\text{O}_3$ interface dipole under gate bias.

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7:50pm PCSI-MoE-5 How to Choose a Gate Dielectric for Rutile GeO_2 , Xiaoru Zhang, The University of Texas at Austin; Alexander A. Demkov, University of Texas at Austin

Electrification, renewable-energy conversion, and data-intensive computing require efficient power electronics at high voltage, frequency, and temperature. Wide-bandgap semiconductors address these needs, while ultrawide-bandgap (UWBG) materials offer still larger breakdown fields [1]. Rutile GeO_2 (r- GeO_2) is an emerging UWBG semiconductor with a ≈ 4.7 eV gap, favorable thermal transport properties, predicted possibility of ambipolar doping, and recent demonstration of single-crystal growth and fabrication of MOSFET [2,3,4]. However, metal-oxide-semiconductor devices require structurally compatible gate dielectrics with sufficiently large barriers to both electron and hole injection. Because r- GeO_2 has a rather wide gap, satisfying both barrier conditions is especially restrictive [5].

We use first-principles calculations to compare r- $\text{GeO}_2(001)$ interfaces with crystalline and amorphous SiO_2 , crystalline and amorphous Al_2O_3 , and crystalline MgO . Amorphous oxides are generated by melt-and-quench molecular dynamics, and representative atomistic models are shown in Fig. 1. Valence-band offsets are independently determined from core-level alignment, electrostatic-potential lineups, and layer-projected densities of states. The conduction-band offsets are then determined using experimental band gaps for dielectrics and ab initio band gaps for r- GeO_2 . All five interfaces exhibit type-I band alignment. MgO and Al_2O_3 show asymmetric carrier confinement, with relatively large electron barriers but comparatively weak hole barriers. SiO_2 provides the most balanced confinement for both carrier types.

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7:55pm PCSI-MoE-6 Study of Metallization-Induced Interface Traps and Charge in $\text{Al}_2\text{O}_3/\text{SiO}_2/\text{Si}$ MOS Stack Using C-V/G-V Measurements and TCAD Simulations, Swadhin Jena, Akshay K., Parlapalli Satyam, IIT Bhubaneswar, India

Atomic layer deposited (ALD) Al_2O_3 on thermally grown SiO_2 as a bilayer stack is emerging as a robust gate dielectric and passivation layer for low-power CMOS, high-power devices, embedded non-volatile memories, emerging 2D-FETs, and PERC solar cells. Because post-deposition annealing (PDA) can damage fragile channel interfaces or exceed the thermal budget of back-end and 3D-sequential integration, the critical bottleneck is the integration of the metal electrode after the dielectric deposition. In this study, we fabricate $\text{Al}_2\text{O}_3/\text{SiO}_2/\text{Si}$ metal-oxide semiconductor (MOS) structures using three different metallization methods, such as thermal evaporation, e-beam evaporation, and sputtering. Using the capacitance-voltage (C-V) measurement technique, we extract and compare the effective oxide-trapped charges (Q_{eff}) and interface trap states (N_{eff}) of samples whose electrodes were deposited using the three methods. Thermal evaporation was found to be the most optimal method, producing the lowest effective oxide charge ($(9.4 \pm 0.2) \times 10^{10} \text{ cm}^{-2}$) and N_{eff} ($(6.6 \pm 0.5) \times 10^{11} \text{ cm}^{-2} \text{ eV}^{-1}$) in the stack. Sputtered metallization resulted in the highest effective oxide charge ($(6.2 \pm 0.5) \times 10^{12} \text{ cm}^{-2}$) and significant border trap charge (Q_{bt}). Notably, the e-beam method also generated high and nearly equal N_{eff} ($\sim 1.5 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$), indicating high near-interface damage. TCAD simulation fitting to experimental C-V data yielded a unique trap

distribution. PMA helps in a significant reduction of generated trap charges, but does not remove them completely. Hence, there is a residual effect of the high-energy metallization method on the $\text{Al}_2\text{O}_3/\text{SiO}_2/\text{Si}$ stack that must be considered in semiconductor design and manufacturing.

8:00pm PCSI-MoE-7 Influence of Ti Adhesion Layer and ALD Al_2O_3 Thickness on Metal/Insulator/Metal (MIM) Interfacial Energy Barriers, *John Conley, Jessica Haglund*, Oregon State University

Understanding and control of interfacial energy barriers (ϕ_{Bn} 's) at metal/insulator contacts is essential for designing MIM and MOS based devices. Interfacial energy barriers are difficult to predict as they depend not only on the metals and dielectrics used, but also on deposition method, deposition order, interfacial interactions such as diffusion and oxygen scavenging, intrinsic and extrinsic defects, and possibly even film thickness. Ultrathin dielectrics are needed for MOS gates and MIM capacitors. It has been reported that the dielectric constant, density, and optical refractive index of ALD Al_2O_3 are a function of film thickness. Thin interfacial metals have been investigated to tailor barrier heights and are required for good adhesion of noble metal electrodes to oxides. In this work, we investigate the impact of Ti adhesion layer (dTi) and Al_2O_3 film (d Al_2O_3) thickness on ϕ_{Bn} 's in bimetal electrode Pt/Ti/ Al_2O_3 /TiN MIM devices using internal photoemission (IPE) spectroscopy.

100 nm TiN bottom electrodes were reactive ion sputtered. Al_2O_3 was then deposited via ALD at 250 °C using TMA / H_2O in either a Picosun R150 or R200 chamber. Following ALD a thin Ti IL (0.5, 1, 2, 5, 10 nm) and a 10 nm Pt top electrode were deposited via electron beam evaporation using a shadow mask. CV and IV measurements were taken on the MIM structures. Energy barriers were measured using a lab-built IPE spectrometer system. Top gate voltage was swept from 0 to ± 2 V using ± 0.1 V steps. At each bias, incident photon energy was swept from 1.7 to 5.5 eV. IPE thresholds (ϕ_{thres}) were determined at each voltage using yield plots and zero field barriers (ϕ_{Bn}) were determined using Schottky plots.

d Al_2O_3 : Impact Both the top Pt/ Al_2O_3 and bottom TiN/ Al_2O_3 electron barriers were found to be a function of d Al_2O_3 . While both barriers were roughly constant at ~ 3.6 eV for Al_2O_3 films ≥ 12 nm thick, both decreased by roughly 0.5 eV as d Al_2O_3 decreased down to 5 nm.

dTi: For bimetal Pt/Ti electrodes, a 0.5 to 1.0 nm thick interfacial Ti layer was found sufficient to completely dominate the barrier with Al_2O_3 . Insertion of the Ti layer resulted in band tailing at the top interface, likely due to oxygen scavenging, but had no impact on the bottom Al_2O_3 /TiN barrier.

The degradation of interfacial energy barriers with Al_2O_3 thickness and the dominant influence of even a very thin Ti interfacial layer on ϕ_{Bn} are important considerations for the prediction and optimization of leakage currents and performance for these devices.

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8:05pm PCSI-MoE-8 Consistency Checks for Semiconductor Contact Extraction, *Dong Kyun Lim, Jin-Hong Park*, Sungkyunkwan University (SKKU), Republic of Korea

Finite-length transmission-line model (TLM) fits can return positive contact parameters despite uncertain geometry or incorrect de-embedding. We present an explicit consistency workflow for extracting specific contact resistivity and under-contact sheet resistance within established finite-contact TLM. For positive, width-normalized, de-embedded contact-front resistances Q_1 and Q_2 at effective lengths L_1 and L_2 , uniform linear-ohmic, one-dimensional transport with equipotential metal and shared positive contact parameters implies $1 < r < k$, where $r = Q_1/Q_2$ and $k = L_2/L_1 > 1$.

A joint (r, k) uncertainty region is screened before inversion. Disjointness from the closed admissible domain indicates inconsistency with the combined model and error assumptions; boundary overlap is inconclusive; a strictly interior region permits conditional inversion. Resistance-geometry covariance can reverse classification in either direction relative to a fixed-geometry ablation at the same cutoff. Transfer-length sensitivity deteriorates near both ratio limits.

Across 1,500 synthetic Gaussian regions, the analytical procedure and a same-information constrained-distance solver gave identical decisions. In a selected synthetic de-embedding-offset example, a noiseless two-length fit

overestimated specific contact resistivity by 16.4% and under-contact sheet resistance by 45.6%. All 30,000 noisy two-length regions were interior, yet a nominal 95% held-out third-length residual test rejected only 6.90%. The workflow makes conditional extractability and its limits explicit; neither an interior result nor agreement at an additional length validates the physical model. No measured device data or inferential superiority are claimed.

8:10pm PCSI-MoE-9 Studying Thin Film Surface & Interface Engineering Using Xps and Strataphi: Depth-Resolved, Non-Destructive Analysis of Layered Materials, *Jia Lu, Norb Biderman*, Physical Electronics USA

The development of next-generation engineered materials demands new approaches. As material systems become more complex, the need for accurate and precise depth-resolved characterization of layered materials becomes critical for understanding the devices' performance, reliability, and process control. *StrataPHI* 3.0 introduces an integrated characterization platform designed for non-destructive, depth-resolved analysis of multi-layer structures composed of ultra-thin layers.

By leveraging data from X-ray photoelectron spectroscopy (XPS) and hard X-ray photoelectron spectroscopy (HAXPES), *StrataPHI* extracts the key processing-dependent material parameters (e.g. layer thickness, composition, and fractional coverage) across the multi-layer stack, from sub-monolayer up to 30 nm below the surface. The newest *StrataPHI* platform also introduces an "integrated analyzer acceptance angle mode (AAA mode)", further strengthens *StrataPHI*'s application in metrology, delivering rapid and reliable thickness measurement using a single take-off angle (TOA).

For ultra-thin films prepared using atomic layer deposition (ALD), the key question is not only how thick the deposited material is, but also how completely it covers the substrate. Traditionally, characterization of fractional coverage of thin films is done by a stand-alone low energy ion scattering (LEIS) instrument for the best sensitivity and peak separation. *StrataPHI* uses XPS peak intensities and attenuation-based thin-film models to simultaneously evaluate thickness and coverage of ALD-deposited layers. *StrataPHI* fraction coverage calculation for Al_2O_3 deposited on SiO_2/Si substrate shows similar values compared to the stand-alone LEIS across multiple ALD cycles.

This poster presentation will demonstrate how *StrataPHI* enables researchers, scientists, and engineers to model complex ultra-thin film structures, providing a deep understanding of the ultra-thin films, surfaces, as well as buried interfaces. With automated batch processing, *StrataPHI* can further link processing conditions to thin-film properties, providing a comprehensive characterization suite for tighter control over performance and reliability of new materials and devices.

PCSI

Room Ballroom - Session PCSI-TuM

Oxides II & Energy Materials

Moderator: Alex Demkov, The University of Texas

8:30am PCSI-TuM-1 Electron-Phonon Interactions in Oxide Materials from First Principles: Implications for Exciton Properties and Superconductivity, **Antonios Alvertis**, University of Texas at Austin INVITED

Polar metal oxides form an ideal testbed for electron-phonon physics. The strong ionic character of these materials produces a stark contrast between the static dielectric constant, which includes ionic contributions, and the high-frequency dielectric constant. This in turn results in significant long-range Fröhlich coupling between charge carriers and longitudinal optical phonons.

In this talk I will explore a number of implications of the long-range electron-phonon interaction in oxides, for superconductivity in SrTiO_3 – a long-standing puzzle for condensed matter theory – and for excitonic effects in a wide range of oxides. I will demonstrate a first-principles theory of superconductivity in SrTiO_3 , which results in good agreement to experiment for the superconducting dome, wherein superconductivity arises from the interplay of the significant Fröhlich interaction with the strong deformation potential coupling associated with the Ti-O bond [1,2].

Apart from mediating the formation of Cooper pairs, as in SrTiO_3 , this interplay of Fröhlich interaction and strong deformation potential coupling that is present in several oxides, can have a strong impact on the excited state properties of these materials. I will present a first-principles theory for including phonon effects in excitonic calculations within the GW-BSE framework [3], and apply it to a range of oxides that include MgO , TiO_2 , BiVO_4 , and SrTiO_3 . I will demonstrate that this results in greatly improved agreement to experiment for a number of quantities, including the exciton binding energy and the optical absorption spectra [3,4].

I will close my talk with a discussion of the validity of perturbation theory for electron-phonon interactions in oxide materials, which is almost universally employed in theoretical studies. I will show that low-order perturbation theory can frequently fail catastrophically, and I will present an approach for incorporating non-perturbative electron-phonon interactions from first principles, which results in large corrections to excited state properties in a wide range of properties, compared to low-order perturbative approaches [5].

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9:00am PCSI-TuM-7 Interfacial Redox Stabilization in High-Entropy Garnet Electrolytes, **Zhezhen Fu**, Fernando Soto, Penn State Harrisburg

Interfacial reduction limits the stability of garnet electrolytes in lithium-metal batteries. Here, we examine how multication substitution regulates redox evolution at the lithium-garnet interface during electrochemical cycling. We compare the high-entropy garnet $\text{Li}_6\text{La}_3\text{Zr}_{0.5}\text{Nb}_{0.5}\text{Ta}_{0.5}\text{Hf}_{0.5}\text{O}_{12}$ (LLZNTN) with conventional Ta-doped $\text{Li}_{6.75}\text{La}_3\text{Zr}_{1.75}\text{Ta}_{0.25}\text{O}_{12}$ (Ta-LLZO), which exhibit comparable room-temperature ionic conductivities. Despite similar initial interfacial resistances, LLZNTN reaches a critical current density of 0.8 mA cm^{-2} , twice that of Ta-LLZO. After critical-current testing, its interfacial area-specific resistance increases from 16 to $20 \text{ } \Omega \text{ cm}^2$, compared with 14 to $75 \text{ } \Omega \text{ cm}^2$ for Ta-LLZO. LLZNTN also sustains stable lithium plating and stripping for 500 h at 0.1 mA cm^{-2} . X-ray photoelectron spectroscopy reveals progressive Ta and Zr reduction in Ta-LLZO during cycling, while reduced Ta, Zr, and Nb components show little further evolution in LLZNTN. Raman spectra indicate better preservation of the LLZNTN garnet framework. Molecular dynamics simulations suggest that cation mixing and surface lithium enrichment limit reactive Li(metal)-O contacts on the modeled (001) interface. These findings support self-limiting reduction in LLZNTN and show that Nb incorporation need not cause progressive degradation. They highlight the local cation environment as a design variable for stabilizing lithium-garnet interfaces.

9:05am PCSI-TuM-8 Ultralow Loading Platinum Films by Direct Atomic Layer Processing for Efficient Hydrogen EvolutionR. Sharma^{1,*,} M. Carnoy¹, M. Ceccato², B. Borie¹, M. Baraket¹, M. Plakhotnyuk¹ ¹Atlant 3d, Mårkærvej 2b, 2630 Taastrup, Denmark² Department of Chemistry and Inano, Aarhus University, 8000 Aarhus C, Denmark, *Ruchi Sharma*, Mårkærvej 2B, Taastrup, DK-2630, Denmark

Platinum provides benchmark hydrogen evolution reaction (HER) kinetics in acid, but reducing noble-metal inventory requires deposition routes that form active, electrically continuous films at ultralow loading. Here, Direct Atomic Layer Processing (DALP), a maskless microreactor implementation of spatial atomic layer deposition, was used to deposit Pt films with nominal thicknesses of 2, 10, 20, 30, and 50 nm directly onto 1 cm^2 glassy-carbon electrodes [1]. The corresponding nominal Pt loadings were 4.29, 21.45, 42.9, 64.35, and $107.25 \text{ } \mu\text{g cm}^{-2}$. Electrochemical performance was evaluated in $0.5 \text{ M H}_2\text{SO}_4$ by cyclic voltammetry and linear-sweep voltammetry, with potentials referenced to the reversible hydrogen electrode. Characteristic hydrogen-underpotential-deposition and Pt oxide-reduction features confirmed electrochemically accessible Pt surfaces. The 2 nm film exhibited a roughness factor of 0.43 and required about 100 mV overpotential to reach 10 mA cm^{-2} . Increasing the film thickness to 10 nm sharply reduced this overpotential to approximately 45 mV and produced the lowest fitted Tafel slope, 21.7 mV dec^{-1} . Films from 20 to 50 nm retained near-zero HER onset, approximately 50-60 mV overpotential at 10 mA cm^{-2} , and Tafel slopes of 26.8 - 33.7 mV dec^{-1} , while additional Pt did not improve benchmark performance proportionally. Thus, the 10 nm film delivered activity comparable to films containing up to five times more Pt, consistent with prior low-loading Pt studies [2]. These results identify film continuity as the key transition from sparse ultralow-loading Pt to an efficient electrode and establish DALP as a digital route for screening and patterning binder-free catalysts with high precious-metal utilization.

Figure 1. DALP Pt deposition and thickness-dependent HER metrics. Overpotentials are approximate values read from the polarization results.

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9:10am PCSI-TuM-9 The Role of Near-Surface Bond Energetics in Shaping Nanoalloy Transformed Configurations, **Micha Polak**, Ben Gurion University of the Negev, Israel

In addition to the surface-layer composition, the subsurface layer in alloy nanoparticles is expected to affect their catalytic activity and selectivity. This theoretical-computational study focuses on the largely unexplored issue of nanoalloy compositional configurations arising from near-surface energetics and involved in thermally induced phase-separation transformations. Employing the statistical-mechanical Free-Energy Concentration Expansion Method (FCEM) [1] with Coordination-dependent Bond-Energy Variations (CBEV) [2] and Effective Pair Interactions (EPI) as part of the input, and the Coarse-Grained Layer Model for additional efficiency, atomic site-specific configurations were computed as a function of temperature for four heterogeneous-catalysis-related binary alloy nanoparticles having relatively small atomic-size mismatch: **Pd-Ir**, **Ag-Ir**, **Pt-Ir**, and **Pd-Rh**, all as 1415-atom cuboctahedrons. We predict distinct inner-core transitions between asymmetric and symmetric configurations beneath a surface-segregated monolayer (Fig. 1): Quasi-Janus (QJ) to solid-solution (SS) in Pd-Ir; QJ to asymmetric core-shell (asy-CS-a), followed by symmetric core-shell (CS-a) in Ag-Ir, and asy-CS-a transformed to CS-a in Pt-Ir and Pd-Rh. To quantify the roles of the CBEV and EPI, we introduce a straightforwardly calculated subsurface/inner-core permutation energy factor (λ) that predicts stable configurations without the need for FCEM computations (and has a clear correlation with the transformation temperature). Thus, its magnitude reflects the identity of the transformed configuration, e.g., for QJ to SS, λ is near zero. Application of the present methodology to ternary, quaternary, and quinary (high entropy) nanoalloys composed of the same elements is underway.

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Fig. 1 Representations of several configuration candidates for the four selected A-Bnanoalloy systems.

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9:15am **PCSI-TuM-10 Hydrogen-Enhanced Schwoebel Barriers and Anisotropic Strontium Diffusion on Vicinal Si(001)**, *Jon Reising, Alexander Demkov*, University of Texas at Austin

Functional oxides such as BaTiO_3 can add electro-optic functionality to silicon devices [1]. Epitaxial integration commonly uses a SrTiO_3 buffer [2–4], initiated by depositing half a monolayer of Sr at 625 °C to protect silicon from oxidation. Growth on vicinal Si(001) substrates [5,6] introduces terraces and steps that complicate Sr migration. We examine how hydrogen affects Sr migration on double-step Si(001) surfaces with a (2×1) reconstruction.

In this talk, we present first-principles calculations for bare and H-passivated surfaces with a 6.8° miscut and 22.59 Å terrace width (Fig. 1). On the bare surface, Sr moves from a terrace trough into a secondary minimum between step-edge dimers before descending. Hydrogen raises the initial barrier toward the step from 0.983 to 1.055 eV and adds two intermediate minima. Our multistate model predicts approximately tenfold slower step crossing. Conversely, hydrogen lowers the barrier along the trough above the step from 0.917 to 0.812 eV, yielding an approximately tenfold faster transition rate.

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9:20am **PCSI-TuM-11 Defect- and Interface-Driven Behavior in Oxide Thin Films**, *Andrew O'Hara*, Western Michigan University **INVITED**

Complex and functional oxides possess a wide range of properties, providing platforms for tunable and emergent behavior via interfaces, defects, and reduced dimensionality. In this talk, I will discuss the effect of defects on magnetic properties and the emergence and role of unique phonons in thin oxide films across multiple theory-experiment collaborations.

Given the sensitivity of oxide magnetism to local crystal structure, growth conditions may lead to unexpected or undesirable outcomes. MBE-grown Co-substituted BaTiO_3 films remain non-magnetic due to oxygen-vacancy-mediated spin coupling. In heterostructures, thin nominally conductive magnetic layers may be especially defect sensitive. In PLD-grown $(\text{SrTiO}_3)^5\text{-(SrRuO}_3)^n\text{-(SrTiO}_3)^5$ films, transport measurements indicate that the $n = 2$ structure is conductive and ferromagnetic, but the $n = 1$ structure is insulating and non-magnetic. STEM imaging reveals Ru-Ti intermixing in the $n = 1$ structure, which DFT shows leads to AFM-like insulating states. For $(\text{CaRuO}_3)^n\text{-(SrRuO}_3)^1\text{-(CaRuO}_3)^n$ films, as n decreases, local structural perturbations near the SRO layer cause an insulating and magnetic state, suggesting an oxide engineering pathway. As another route, DFT predicts that carrier doping can couple magnetic and polar behavior, enabling switchable spin textures in $\text{h-LuFeO}_3/\text{MnSTe}$.

As in the examples above, decreasing superlattice thickness can also lead to emergent phonon behavior. In PLD-grown $(\text{SrTiO}_3)^n/(\text{CaTiO}_3)^n$ superlattices, STEM imaging and spectroscopy along with optical spectroscopy measurements show the emergence and eventual dominance of interfacial vibrational modes with decreasing n . These observations were corroborated by DFT calculations to understand structural changes and potential defect effects on phonon mode localization. Similar techniques were used to probe related systems like grain boundaries. The role of phonons in the non-resonant excitation and temperature dependence of emission in optically active Er_2O_3 films and how modifying the phonons may affect emission will be discussed.

Defects, interfaces, and reduced dimensionality are not just perturbations to ideal behavior, but ingredients that either prevent or enable unique properties, with their control providing routes to engineering functionality.

PCSI

Room Ballroom - Session PCSI-TuE

Evening Special Session - Whither Majorana?

Moderator: Valla Fatemi, Cornell University

7:00pm **PCSI-TuE-1 Two-Level Systems, Quasiparticles, and Decoherence of Majorana Qubits in Super-Semiconducting Hybrid Structures**, *Susan Coppersmith*, University of New South Wales, Australia **INVITED**

Qubits based on Majorana zero modes (MZMs) in superconductor–semiconductor heterostructures have attracted intense interest due to claims that their topological protection will ensure extremely high qubit fidelities [1]. However, our work shows that current experiments realizing these qubits in InAs heterostructures are subject to substantial decoherence resulting from the high-frequency components of the fluctuations of two-level systems (TLSs) that are ubiquitous in the materials surrounding the nanowire [2,3]. This process excites quasiparticle pairs in the bulk of the topological superconductor that cause qubit decoherence even under otherwise ideal conditions. Increasing nanowire capacitance suppresses this mechanism but exposes the qubits to decoherence from externally-generated quasiparticles. Therefore, achieving high-fidelity MZM qubits using superconductor–semiconductor nanowires will require engineering strategies and compromises very similar to those needed for other solid state qubits.

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7:30pm **PCSI-TuE-7 Invited Paper**, *Greg Mazur*, University of California Santa Barbara

PCSI

Room Ballroom - Session PCSI-WeM1

2D Materials: Graphene & Beyond

Moderator: Jun Xiao, University of Wisconsin - Madison

8:30am PCSI-WeM1-1 Unconventional Domain Tessellations in Moiré-of-Moiré Lattices, *Hyobin Yoo*, Seoul National University, Republic of Korea

INVITED

Twisted trilayer van der Waals crystals enable the creation of hierarchical moiré-of-moiré lattices by overlapping two moiré patterns through controlled twist angles. At small twist angles, the interlayer and intralayer interactions at two distinct interfaces in the twisted trilayer crystals give rise to an intricate network of domain structures that exhibit exotic electronic properties. In this study, we present a comprehensive structural phase diagram of twisted trilayer graphene (TTG) with atomic-scale lattice reconstruction. Using transmission electron microscopy in conjunction with advanced interatomic potential simulations, we reveal a variety of large-scale moiré lattices, including triangular, kagome, and hexagram-shaped domain patterns.[1] Each domain is enclosed within a two-dimensional network of domain wall lattices. At small twist angles, competing rhombohedral and Bernal stacking orders, separated by a small energy difference, induce unconventional lattice reconstructions characterized by spontaneous symmetry breaking and nematic instability, emphasizing the role of long-range interactions across van der Waals layers.[1] The tunable tessellation of diverse domain networks by adjusting the twist angles establishes TTG as a versatile platform for investigating the relationship between engineered nontrivial domain lattice structures and their emergent physical properties.

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9:00am PCSI-WeM1-7 UPGRADED: Unusually Strong Electron-Phonon Kinks in Graphene and hBN, *Justin Wells*, University of Oslo, Norway

In 2013, we controversially reported strong electron-phonon coupling (EPC) in graphene's σ -bands [PRL 111:216806]. The result was controversial. Combining theoretical support with measurements in neighbouring Brillouin zones, we showed that the mass enhancement, $\lambda \approx 0.7$, was intrinsic [PRB 95:075430].

We subsequently predicted similarly strong EPC in the σ -bands of hBN [PRB 101:214513], whose electronic and phonon structures resemble those of graphene. Experimental confirmation further supported our understanding of EPC in graphene. Unlike graphene, hBN was predicted to exhibit strong EPC in its π -band, whose parabolic maximum leads to fundamentally different scattering phase space and much stronger coupling.

Most recently, we have developed improved our mathematical tools for analysing EPC. Established methods are implicitly based on the assumption of linear electronic bands, and are unsuitable near a parabolic maximum.

We reveal that π -band EPC depends strongly on doping, substrate choice and substrate interaction strength. In this talk, I will show our latest studies and analysis, as well as the open question which motivate ongoing ARPES, DFT and helium-scattering studies.

9:15am PCSI-WeM1-10 Self-Intercalated Ti Reveal Stacking Order in Bilayer TiSe₂ Films, *Nicolas Paulo Pereira Vasconcelos*, University of South Florida

Alternatively stacked transition metal dichalcogenides (TMD) may give rise to properties distinct from those of their conventional structures. Different layer stacking can also originate distinct point defects. Proper identification of defects is therefore important for the understanding of the properties of these materials. Here, scanning tunneling microscopy was used to identify native defects in MBE-grown ultrathin TiSe₂ and to investigate the coexistence of an alternative stacking configuration. In monolayers surface and sub-surface Se-vacancies dominate. In bilayers, two additional point defects are observed that are separated into domains and are interpreted as Ti self-intercalation defects. The conventional 1T-TiSe₂ stacking cannot account for both defect configurations, suggesting the existence of an alternative stacking. Rotating the top layer 180° about an axis passing through a Se atom at the bottom of the top layer. results in the alternative stacking. In both stacking configurations self-intercalated Ti atoms can occupy the preferred octahedral site, but express different symmetries allowing for discrimination between the stacking in STM images. Finally, sequential thermal annealing revealed a local structural transformation associated with increase of Ti intercalation, forming an irreversible 2x2-like periodic superstructure.

Wednesday Morning, January 20, 2027

9:20am PCSI-WeM1-11 Electronic Spectroscopy of Atomic Defects in Molybdenum Disulfide under Ambient Conditions, *Joshua R. Evans*, *Diego A. Garibay*, *Aiden N. Kuhls*, *Mehmet Z. Baykara*, University of California at Merced

Two-dimensional transition metal dichalcogenides (2D-TMDs) are promising candidates for next-generation, nanoscale electronic devices due to their profound optoelectronic properties (e.g., direct and tunable bandgaps) [1]. However, these materials host atomic-scale defects (e.g., vacancies, substitutions, etc.), introducing electronic heterogeneities that can either enhance or hinder device performance [2], [3]. Thus, characterizing atomic defects within 2D-TMDs is essential for nanoscale device implementation. Current-voltage (I-V) spectroscopy via conductive atomic force microscopy (C-AFM) characterizes electronic properties under ambient conditions [4]. Thermal drift makes this method unsuitable, reducing confidence in assigning electronic features to specific defects. We present an alternative approach on molybdenum disulfide (MoS₂), a representative 2D-TMD, that overcomes thermal drift [5]. Consecutive current maps are collected at various bias voltages, enabling direct assessment of electronic features for defects spanning single atomic sites to several nanometers. Spectroscopy data allows sorting defects into distinct groups, leading to their chemical identification.

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[5] J. R. Evans, D. A. Garibay, A. N. Kuhls, and M. Z. Baykara, "Electronic Spectroscopy of Atomic Defects in Molybdenum Disulfide under Ambient Conditions," *ACS Omega*, in press, 2026.

9:25am PCSI-WeM1-12 Sulfur Vacancy-Induced Dielectric Screening Crossover in Single-Layer WS₂, *Christopher Smyth*, Sandia National Laboratories; *Alex Boehm*, SNL New Mexico - Albuquerque; *Hayden Barry*, University of Virginia, Department of Materials Science and Engineering; *Andrew Kim*, Sandia National Laboratories; *Catalin Spataru*, Sandia national laboratories; *Jordan Hachtel*, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory; *Tzu-Ming Lu*, Sandia National Laboratories; *Jose Fonseca*, *Jeremy Robinson*, Naval Research Laboratory; *Kory Burns*, University of Virginia; *Taisuke Ohta*, Sandia National Laboratories

Dielectric property in two-dimensional (2D) semiconductors is set by the external environment, charge carriers, and disorders, making defects a tuning parameter to modulate their electronic response. Here, we reveal quasiparticle electronic band gap ($E_{g,QP}$) renormalization in single-layer (1L) WS₂ by independently tuning sulfur vacancy density and substrate screening. Photoelectron spectroscopy and electron energy loss spectroscopy show that a defect density (ρ) of reduces $E_{g,QP}$ from 2.4 eV to 2.2 eV in weakly-screened, suspended WS₂ with the diminished exciton binding energy (E_b) by 0.2 eV. In Au-supported WS₂ with strong external screening, $E_{g,QP}$ remains ~ 2.0 eV showing no $E_{g,QP}$ renormalization upon increasing ρ . Enhancing disorder additionally drives the reduced photoelectron core-hole relaxation in suspended WS₂ when the exciton screening length (estimated from E_b) exceeds the mean interdefect spacing of ~ 4 nm at ρ . This threshold signifies the crossover from weak to strong polarizability in 2D dielectric screening.

9:30am PCSI-WeM1-13 Information-Theoretic Imaging of Layered Quantum Materials, *Monica Allen*, University of California at San Diego

INVITED

Scanning microwave impedance microscopy (MIM) probes the local complex conductivity of a material, providing a spatially resolved view of electronic states and their evolution. In recent years, MIM has emerged as a powerful tool for investigating topological phases and correlated quantum matter. In this talk, I will discuss new approaches that extend the information accessible through the microscopy of quantum materials. First, I will describe a layer-resolved imaging technique that resolves electronic states on individual atomic planes within van der Waals heterostructures at temperatures down to 50 mK. By visualizing charge disorder across

8:30 AM

different atomic layers, we investigate how surface impurities and electrostatic screening influence the formation of fractional quantum Hall states. I will then discuss an approach that combines microscopy with tools from information theory to quantify spatial complexity and hidden order directly from images. Together, these developments illustrate how spatially resolved measurements can provide new perspectives on disorder, quantum criticality, and the microscopic nature of electronic phase transitions.

PCSI

Room Ballroom - Session PCSI-WeM2

Molecular, Organic and Hybrid Interfaces

Moderator: Noa Marom, Carnegie Mellon University

11:00am **PCSI-WeM2-31 UPGRADED: Direct Writing of N-Heterocyclic Carbene Nanostructures**, Milan Kubicki, Technische Universität Berlin, Germany; Preeti Chahar, Universität Münster, Germany; Dominik Schmidt, Technische Universität Berlin, Germany; Ankita Das, Universität Münster, Germany; Marie-Louise Fraser, Anna Doronina, Gustav Lorenz, Clara Kühn, Johannes Troger, Philipp Gruber, Viktoria Balfanz, Mario Dähne, Technische Universität Berlin, Germany; Conor Hogan, CNR-Istituto di Struttura della Materia (CNR-ISM), Italy; Frank Glorius, Universität Münster, Germany; **Martin Franz**, Technische Universität Berlin, Germany

To date, various scanning probe lithography (SPL) techniques already exist, in which scanning probe microscopes are used to directly create nanostructures on surfaces. Thereby, different physical and chemical effects are used to locally change the structure of the sample surface beneath the probe. Examples include thermal or thermochemical SPL, oxidation SPL, and dip-pen nanolithography [1].

Here, we present a method allowing the direct writing of nanostructures consisting of monolayers of N-heterocyclic carbene (NHC) molecules. NHCs constitute a well-established class of organic compounds with applications in homogeneous catalysis, main-group chemistry, and functional materials [2]. In recent years, they have also emerged as important ligands for surface modification and functionalization. While initial research focused mainly on noble metal surfaces, other substrates such as semiconductors have recently come into focus [3,4].

In the NHC-SPL method demonstrated here, the writing is induced by the electric field between the STM tip and the surface, thus it can be regarded as a sort of bias-induced SPL. During writing, molecular precursors, which are present on the surface as a highly mobile molecular gas are attracted towards the tip-sample gap and immobilized underneath the tip. This is accompanied by a covalent bonding to the surface resulting in the formation of highly stable NHC monolayers. The method allows for the creation of arbitrary structures with resolutions in the range of single nanometers. The writing furthermore works on a variety of (modified) semiconductor surfaces and with different NHC molecules, making a wide range of applications conceivable.

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11:15am **PCSI-WeM2-34 UPGRADED: Is the CISS Effect a Special Case of Emergent Magnetization at Metal-Molecule Interfaces?**, Yonatan Dubi, Ben Gurion Uni. Be'er Sheva, Israel

Chirality-induced spin selectivity (CISS) is the magnetically non-trivial electronic response of chiral molecules: the current through a chiral molecular junction depends on the magnetization of a ferromagnetic electrode and on handedness, and electrons photoemitted through a chiral layer emerge spin-polarized, with a sign set by handedness [1]. The effect is large and survives at room temperature. The origin of the CISS effect is a major open question, but experimental evidence point strongly to an interface effect [2].

The "Spinterface mechanism" [1,3] suggests that the CISS is an interface phenomena. It relies on an assumption (motivated by the appearance of magnetization in metal-molecule hybrid systems discussed above) that the interface between the metal and molecule gives rise to some localized magnetic moment, whose direction is undetermined. The adsorption of a chiral molecule drives a transient charge redistribution in a chiral environment, accompanied by a pulse of magnetic field along the chiral

axis; with exchange coupling and dissipation into the metal, this stabilizes the fluctuating surface moments along that axis. This is the only theoretical approach to CISS that permits *direct fitting of raw experimental data* [3].

This is not the only magnetic effect arising in hybrid metal-molecule interfaces. In fact, evidence for magnetic effects in hybrid interfaces with *achiral* molecules is over two decades old [4]. And yet, to the best of our knowledge, no one in the CISS or other community has made the connection between the two.

In this talk we demonstrate that the "spinterface mechanism" provides a direct and natural link between these two families of phenomena. The magnetism arises from the same reasons, namely the presence of magnetic moments at the metal-molecule interface, and chirality is a *director* for the effect, supplying an out-of-plane advantage that prevents cancellation that typically washes out the effect in achiral molecules. Thus, CISS may thus be a legible case of emergent interfacial magnetization, and not a unique effect.

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11:30am **PCSI-WeM2-37 UPGRADED: Stable Covalent Bonding between Two Closed-Shell Atomic Orbitals**, Andrés Pinar Solé, Center for Quantum Nanoscience, Republic of Korea

Interactions between two fully occupied atomic orbitals are conventionally expected to be repulsive because both the bonding and antibonding molecular orbitals are occupied, resulting in zero bond order[1]. Here, we demonstrate that proximity to a metallic substrate can qualitatively alter this picture and stabilize a covalent interaction between two atoms with closed-shell valence orbitals. Using scanning tunnelling microscopy, atom manipulation, inelastic electron tunnelling spectroscopy, and first-principles calculations, we investigate Ho dimers manually assembled on two monolayers of MgO on Ag(100). Individual Ho atoms possess fully occupied, atomic-like 6s orbitals and show no spin excitations within the investigated energy range[2][3]. In contrast, Ho dimers exhibit intense spin-flip excitations between approximately 60 and 130 meV. The spatial distribution and energy of these excitations, combined with electronic-structure calculations and a tight-binding model, identify an unpaired electron in an antibonding molecular orbital derived predominantly from the Ho 6s states. We show that formation of this state results from partial depopulation of the antibonding orbital through coupling to the metallic substrate. The resulting imbalance between bonding- and antibonding-state occupations produces a net attractive covalent interaction despite the closed-shell character of the isolated atoms. Furthermore, changing the adsorption-site coordination modifies atom-substrate hybridization and systematically tunes the spin-flip excitation energy. These results reveal a substrate-enabled mechanism for covalent bond stabilization between surface adsorbates and illustrate how interfaces can fundamentally modify chemical bonding at the atomic scale.

[1] Pauling, L. Atomic Radii and Interatomic Distances in Metals. *Journal of the American Chemical Society* **69**, 542–553 (1947).

[2] Singha, A. et al. Spin Excitations in a 4 f – 3 d Heterodimer on MgO. *Phys. Rev. Lett.* **121**, 257202 (2018).

[3] Natterer, F. D. et al. Reading and writing single-atom magnets. *Nature* **543**, 226–228 (2017).

11:45am **PCSI-WeM2-40 Rare Earth Modified Silicon Surfaces: A Promising Template for Ordered Organic Growth**, Milan Kubicki, Martin Franz, Mario Dähne, Yi Lu, Marie-Louise Fraser, Philipp Gruber, TU Berlin, Germany

The self-assembly of organic molecules into ordered layers on solid surfaces is of considerable interest for potential applications in advanced optical and electronic devices. While ordered molecular growth on metal surfaces is well established, comparatively little attention has been paid to silicon, which remains the predominant material in modern semiconductor technology. On pristine silicon surfaces, the high density of dangling bonds typically impedes the formation of well-ordered organic films, making appropriate surface modification essential.

Here, we demonstrate that rare-earth-modified Si(111) surfaces provide suitable templates for ordered molecular growth [1]. Using scanning tunneling microscopy (STM) at room temperature, we investigated the adsorption behavior of organic molecules with widely differing degrees of chemical reactivity. These include highly reactive N-heterocyclic carbenes (NHC), moderately reactive PTCDA molecules, and weakly interacting transition metal phthalocyanines. At submonolayer coverages, most molecules remain mobile on the surface, whereas highly ordered films form at monolayer coverage for all systems investigated. Figure 1 shows representative STM images of the ordered structures formed by IPr-NHC, PTCDA, and cobalt phthalocyanine. In all three cases, the molecules form highly ordered commensurable monolayers, with the corresponding periodicities indicated in the STM images.

These findings establish rare-earth-modified silicon surfaces as promising templates for the growth of ordered organic thin films and demonstrate their suitability for molecular layers with markedly different chemical reactivities.

[1] M. Kubicki, M. Franz, and M. Dähne, *J. Phys. Chem. C* **128**, 13347 (2024).

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11:50am **PCSI-WeM2-41 Reversible Subsurface Diffusion and Redox Reactions of 2D Copper Boride**, *Kevin Sutherland*, UC Merced; *Dahee Lee*, *Jennifer Sanchez*, *Adam Buratowski*, University of Texas at San Antonio; *Ashley Head*, *Abdullah Al-Mahboob*, *Dario Stacchiola*, Brookhaven National Laboratory; *Fang Xu*, University of Texas at San Antonio

Boron exhibits exceptional chemical stability, making it an attractive material for applications in catalysis and energy storage [1]. This stability arises from its strong covalent bonding, which makes elemental boron highly resistant to oxidation. When oxidized to boron oxide (B_2O_3), it is thermodynamically stable and difficult to reduce, even in reducing environments such as CO or hydrogen. 2D boron, which is characterized as borophene or a transition metal boride, depending on the substrate, is often grown on Cu(111) [2]. There is limited knowledge in the current literature regarding the chemistry of 2D boron. However, partially oxidized 2D copper oxide species are considerably more reactive and can be reduced more readily than fully oxidized 2D copper oxide [3]. This same concept can be applied to partially oxidized 2D boron. Despite the importance of these oxidation states, their formation and evolution have received little attention for 2D boron surfaces. Understanding the oxidation process is therefore critical for controlling the chemical stability, reversibility, and performance of 2D boron, motivating the investigation of early stage oxidation presented herein.

2D B/Cu(111) synthesis was first optimized by post annealing while recording in-situ low energy electron microscopy (LEEM) and low energy electron diffraction (LEED) data. The results were confirmed with scanning tunneling microscopy (STM) (Fig. 1) and auger electron spectroscopy (AES). Boron deposition on Cu(111) produced a clean 2D copper boride film through reversible diffusion between the surface and subsurface. Oxidation experiments revealed the reaction pathway in which copper boride first forms partially oxidized boron oxide (Fig. 2), reacts preferentially with water at elevated temperature to produce boric acid, and subsequently dehydrates into stable B_2O_3 upon reduction with CO.

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PCSI

Room Ballroom - Session PCSI-WeA1

Topological Thin Films & Heterostructures

Moderator: Cui-zu Chang, Penn State University

2:00pm PCSI-WeA1-1 From Epitaxy to Emergent Properties in Topological Quantum Materials, **Matthew Brahlek**, Oak Ridge National Laboratory

INVITED

Interfacing topological materials with other functional materials offers promising platforms for realizing and manipulating novel quantum phenomena, yet their properties are often limited by defects [1], which are compounded by complex materials processing at epitaxial interfaces. Molecular beam epitaxy (MBE) gives the highest level of control over thin-film synthesis, including composition, thickness, substrate termination, strain, and interfacial structure. I will discuss how this high level of control can enable the integration of topological materials with magnetism and superconductivity. Examples include epitaxial MnBi₂Te₃ [2], where thickness and growth conditions reveal the relationship between intrinsic magnetism, defects, and anomalous Hall response, and Fe(Te,Se)/Bi-Te heterostructures [3-4], where engineered interfaces enhance superconductivity in low-dimensional films. I will also highlight how MBE can suppress structural defects in Bi₂Se₃ [5] and selectively stabilize distinct polymorphs of the novel magnetic material MnTe [6]. Together, these results demonstrate how MBE enables both deeper understanding and deliberate design of emergent properties in topological quantum materials.

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[6] Chen, A.-H., et al. "Programmable Phase Selection between Altermagnetic and Noncentrosymmetric Polymorphs of MnTe on InP via Molecular Beam Epitaxy." *ACS Applied Materials & Interfaces* **18**, 15654–15664 (2026) <https://doi.org/10.1021/acsami.5c14582>

2:30pm PCSI-WeA1-7 UPGRADED: **Negative Longitudinal Magnetoresistance and Angle Dependent Transport Near the Quantum Limit in Cd₃As₂ Films**, **Ian Leahy**, **Anthony Rice**, National Laboratory of the Rockies; **Herve Ness**, King's College London, UK; **Jocienne Nelson**, **Mark van Schilfgaarde**, **Kirstin Alberi**, National Laboratory of the Rockies

The field angle dependence of magnetoresistance (MR) in topological semimetals can contain information about mobility anisotropy and topological transport [1-4]. Here, we report on angle dependent magnetotransport in (001)-oriented Cd₃As₂ thin films with ultralow carrier densities (~2.5 × 10¹⁶ cm⁻³) near their quantum limit. With increasing field magnitude, we identify a striking crossover in the H||I transport from negative longitudinal MR to a huge positive longitudinal MR with magnitude comparable to the transverse MR (Figure 1). Using systematic transport measurements and theoretical modeling of the transport with an 8 × 8 k-p model, we identify a unique quantum-limit contribution governed by Fermi surface anisotropy. We discuss these results within the context of previously undescribed field-angle dependent quantum limit transport in other semimetals.

References:

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2:45pm PCSI-WeA1-10 Thickness-Dependent Fermi Surface Evolution in Ultrathin Bi_{0.85}Sb_{0.15} Films Probed by Shubnikov-de Haas Oscillations, **Shirshendu Chatterjee**, University of California at Santa Barbara

Bi_{1-x}Sb_x was the first experimentally identified three-dimensional topological insulator, hosts spin-momentum-locked surface states protected by time-reversal symmetry [1,2]. Its high mobility and large spin Hall angle make it attractive for spin-orbit-torque devices [3]. In ultrathin films, surface-state hybridization opens a gap [4], quantum confinement forms subbands, and the interfacial asymmetry induces Rashba splitting [5]. As a result, the conducting channels and their Fermi surfaces are expected to depend strongly on thickness in the few-bilayer (BL) range.

This work uses Shubnikov-de Haas (SdH) oscillations to track the Fermi surface of Bi_{0.85}Sb_{0.15} films from 2 BL to 10 BL grown on InSb(111)B. The native oxide on the InSb(111)B substrate was removed by annealing with an impinging atomic H-flux at 300 °C in ultrahigh vacuum (UHV), giving a (3×3) surface reconstruction. The surface was subsequently exposed to an Sb₄ flux to mitigate In droplet formation, followed by annealing to obtain the well-ordered (3×3) surface reconstruction. BiSb was grown on this surface by MBE with the substrate held at room temperature, and then post-growth it was annealed at 80–120 °C for 1h, forming a (1×1) surface reconstruction. Growth was monitored by RHEED, and surface morphology was characterized by STM [Fig. 1(a)]. Hall bars with a channel length of 20 μm and width of 5 μm were fabricated to minimize geometric effects and enable accurate magnetotransport measurements. SdH frequencies, effective masses, and tilt-angle dependence together assign each oscillation to a specific channel (hybridized surface state, confined subband, or interface state). At 2 BL, an increase in resistance to the MΩ range at 1.8 K, together with STM evidence of island formation, indicates incomplete film coalescence and substrate-dominated transport. The challenges of achieving continuous films in this ultrathin limit, and the growth optimizations addressing them, will be discussed. The 3 BL film lies between the hybridization-gapped 2 BL and effectively gapless 4 BL regimes [4]. In this film, R_{xx} shows multiple distinct SdH frequencies [Fig. 1(b,c)] with effective masses of ≈ 0.30, 0.35, and 0.34 m_e. The nearly equal masses of the latter two disfavor independent Dirac pockets and point to spin-split contours of a single band. The full thickness series will show how the Fermi surface pockets evolve from the hybridized to the topological regime, with implications for engineering transport channels in BiSb-based spintronic devices.

2:50pm PCSI-WeA1-11 Classification of Band Topology from Wannier Functions and Tight-Binding, **Jing Zhang**, Imperial College London, UK

Topological insulators present an obstruction to the description of connected bands by Wannier functions in real space. Starting with a set of Wannier functions, the electronic dispersion can be obtained using tight binding (TB) methods. In the case of gapped systems under such description, there is no obvious ways of distinguishing if the connected valence/conduction bands have trivial or non-trivial topology.

Symmetry techniques are developed to identify connected bands with trivial topology, leaving others as symmetry indicated as having non-trivial topology. A key aspect of the symmetry analysis requires the recognition of the **orientability** of the Brillouin zone (BZ) (torus). The BZ of the honeycomb lattice is illustrated in Fig.1. Such orientation changes under some space group operations. The presence of such operations in the space group forbids topological invariants, such as Chern numbers, in connected bands with an invariant band description induced from Wannier functions. This gives rise to the basic selection rule on the topological invariants in connected bands with invariant band description. Connected bands without an invariant band description under TB are symmetry-indicated as having non-trivial topology. The hierarchy of connected band in terms of Wannier function description is shown in Fig.2

Under the TB model, the obstruction to real-space Wannier function description manifests as a lack of invariant band description of the connected bands. The configuration of band connectivity of connected bands with trivial/non-trivial topology is established from Wannier functions using the projection operator technique and provides the corresponding classification of band topology.

The TQC criteria of classifying topological phases are modified from “having atomic limit” to “having an invariant band description induced from Wannier functions”. In turn, Wannier functions, single or multi-centred, can only be defined from Fourier transform of connected bands with trivial topology.

The analysis is illustrated with the honeycomb lattice (graphene). Earlier work was reported in PCSI49.

2:55pm PCSI-WeA1-12 THz Electrodynamics in 2D Correlated Topological Semimetals: From High-Performance Sensing to Programmable Chiral Charge Order, Jun Xiao, University of Wisconsin - Madison INVITED

Two-dimensional correlated topological semimetals provide a unique platform in which strong electron correlations, nontrivial band topology, and broken symmetries converge to generate exceptionally strong nonlinear electrodynamics in THz regime. In the first part of the talk, I will introduce our recent experimental effort to study the unique interplay among the quantum geometrical properties, gate-tunable electron correlation and THz electrodynamics in 2D correlated topological semimetals TaIrTe₄. Building upon the nonlinear Hall effect as a new mechanism for THz rectification, we have observed a large zero-bias responsivity (~ 0.3 A/W), ultralow NEP ($\sim$ pW/Hz^{1/2}), broadband THz response (0.1 to 10 THz) and ultrafast intrinsic speed ($\sim$ ps) at room temperature. The THz sensing performance can be further enhanced by introducing gate-tunable electron correlations [1].

Building on this strong THz light-matter interaction, we explore whether light can move beyond probing electronic order to actively program it. We will discuss how helical optical and THz fields provide a route to reshape this delicate energy landscape, stabilize chiral charge order, and on demand control its handedness [2]. The observed light-induced chiral charge order intertwined with electron correlation and topology establishes the necessary symmetry-breaking conditions to access more exotic phases, such as fractional quantum anomalous Hall states and chiral superconductivity. Together, these results establish THz electrodynamics in 2D correlated topological semimetals as a pathway from high-performance sensing to the programmable creation and control of chiral quantum order.

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PCSI

Room Ballroom - Session PCSI1-WeA2

Thermal Transport, Surface Processing & Nanofabrication

Moderator: Andrew O'Hara, Western Michigan University

4:30pm PCSI1-WeA2-31 Pressure Dependence of Thermal Boundary Conductance at 2D-Substrate Interfaces, Sylvester Makumi, Aidan Belanger, Zlatan Aksamija, University of Utah

Two-dimensional (2D) materials such as graphene and transition metal dichalcogenides (TMDs) offer transformative potential for scaled nanoelectronics, but severe thermal dissipation bottlenecks arise at van der Waals (vdW) interfaces with dielectric substrates. Gate-induced electrostatic pressure (P_{elec}) provides a promising contact-free mechanism to actively modulate thermal boundary conductance (TBC) across these interfaces without inducing mechanical damage [1]. In this study, we present a comprehensive multiscale numerical framework coupling Density Functional Perturbation Theory (DFPT) calculations with phonon transport modeling to elucidate the physical mechanisms governing pressure-enhanced TBC across 2D-substrate interfaces.

Interfacial vdW interactions between 2D sheets and amorphous SiO₂ substrates were calculated from first principles using Density Functional Theory (DFT) implemented in VASP, then parameterized using a modified Buckingham potential fitted to DFT energy-distance curves, yielding precise vdW spring coupling constants $K_s(h)$. Our model incorporates localized surface roughness statistics (RMS height Δ_{rms} , auto-correlation length L_{cor} , and average surface slope of the roughness $\Delta_{\text{rms}}/L_{\text{cor}}$), energy minimization,

and full flexural phonon density of states. On flat substrates, TBC enhancement (dG/dP) is driven exclusively by vdW bond compression, yielding pressure sensitivities of dG/dP = 0.016 ms⁻¹K⁻¹ for unencapsulated graphene/SiO₂ and 0.025 ms⁻¹K⁻¹ when encapsulated, eliminating internal flexural phonon bottlenecks.

When realistic substrate roughness is introduced, partial delamination occurs at zero external pressure, suppressing initial conductance G_0 . Applied electrostatic fields draw suspended regions toward the substrate, expanding the real contact area $\Delta A/\Delta P$ and simultaneously stiffening interfacial vdW bonds $\Delta K_s/\Delta P$ at contact peaks. Consequently, dG/dP exhibits a non-monotonic dependence on surface slope, peaking sharply at $\Delta_{\text{rms}}/L_{\text{cor}} \approx 0.1$, where contact area expansion and bond compression each contribute $\sim 50\%$ to overall TBC enhancement. Beyond this threshold, severe delamination reduces G_0 , suppressing pressure sensitivity. Furthermore, stronger interfacial adhesion increases G_0 and consequently dG/dP, whereas stiffer 2D materials (higher bending stiffness D_{bend}) resist conforming to rough surfaces, creating air gaps that lower TBC. Gate-induced carrier densities up to 2×10^{13} cm⁻² enhance flexural (ZA) phonon repopulation via electron-phonon coupling ($\Gamma_{\text{el-ph}}$), adding $\sim 4\%$ to total TBC [5]. These findings establish key predictive guidelines for active thermal management in 2D electronics.

4:35pm PCSI1-WeA2-32 Tuning the Vibrational Density of States of van der Waals Heterostructures for Enhanced Thermal Boundary Conductance, Aidan Belanger, Sylvester W. Makumi, Zlatan Aksamija, University of Utah

Heterostructures of two-dimensional (2D) vdW materials have emerged as a platform for novel nano- and opto-electronic applications because they offer numerous stacking combinations that may lead to properties not achievable in individual layers. However, the thermal properties of these heterostructures have received less attention, even though they are essential, as Joule heating can generate hotspots in such devices. In 2D transistor applications, hexagonal boron nitride (hBN) is typically used as an interlayer between the 2D channel and the substrate to enhance electron mobility [1] and contribute to heat spreading. Heat transfer between 2D materials and their substrates is driven by a combination of the overlap of the vibrational density of states (vDOS) of the flexural phonons in the 2D layer and the substrate [2,3,4] and vdW coupling strength at the interface. When a 2D layer is coupled to a substrate, the interfacial restoring force opens a gap in the vDOS, with the gap frequency determined by the interfacial force constant and the layer's mass density [5], and when multiple layers are added to the structure, the phonon branches become hybridized [6], creating new features in the vDOS. Whether one can control the vDOS of the heterostructure by selecting the composition and the stacking order in the vdWH to enhance heat transfer to the substrate remains an open question.

In this work, we compute phonon dispersions from density functional theory for the constituent monolayers and construct a coupled dynamical matrix for the out-of-plane flexural phonon branches. We also compute the van der Waals spring constants for the interlayer and substrate interactions. We then calculate the layer-projected vDOS to determine how modes originating in the transport layer contribute to motion in the substrate-interface layer and obtain the thermal boundary conductance (TBC) into the substrate. We observe that coupling to the substrate through long-wavelength breathing modes that displace all layers of the vdW heterostructure dictate the TBC.

[1] H. Y. Lan, R. Tripathi, J. Appenzeller, and Z. Chen, IEEE Electron Device Lett. **45**, 1337 (2024). [2] J. H. Seol, I. Jo, A. L. Moore, L. Lindsay, Z. H. Aitken, M. T. Pettes, X. Li, Z. Yao, R. Huang, D. Broido, N. Mingo, R. S. Ruoff, and L. Shi, Science **328**, 213 (2010). [3] C. J. Foss and Z. Aksamija, 2D Mater. **6**, 025019 (2019). [4] G. C. Correa, C. J. Foss, and Z. Aksamija, Nanotechnology **28**, 135402 (2017). [5] B. Amorim and F. Guinea, Phys. Rev. B **88**, 115418 (2013). [6] Z.-Y. Ong, Phys. Rev. B **95**, 155309 (2017).

4:40pm PCSI1-WeA2-33 The Effect of Surface Roughness on the Interfacial Defect Density between High-k and Silicon Channel of GAAFETs, Seonghwan Shin, Electronics and Telecommunications Research Institute (ETRI), Republic of Korea

Selective removal of sacrificial SiGe is a key step in forming suspended Si nanosheet channels in gate-all-around FETs (GAAFETs). As devices scale down, isotropic chemical dry etching (CDE) is increasingly adopted for channel release [5,6], while wet chemistries suffer from stiction and pattern collapse in narrow gaps [6]. The exposed Si becomes the channel and the gate-dielectric interface, so release-induced damage maps directly onto the interfacial defect density (D_{it}) and subthreshold swing. Here we compare

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dry- and wet-released surfaces and provide a recovery solution based on sacrificial thermal oxidation.

Two candidates can degrade the interface: *atomic-scale roughness* and *residual fluorine*. CDE (a bias-free $\text{CF}_4/\text{O}_2/\text{N}_2$ plasma) attacks the exposed Si once the SiGe is cleared [1,2], whereas wet release (peracetic acid with buffered oxide etchant) proceeds through oxidation of Ge-containing bonds and fluoride-assisted dissolution [3,4]. AFM quantifies the morphological imprint (Fig. 1a): R_q reaches 1.79 nm after 30 s of CDE (16 times the wet value) and keeps increasing during over-etch, whereas wet-released Si stays near 0.1 nm even after 210 s. XPS isolates the chemical imprint (Fig. 1c): only dry-released Si shows an F 1s peak at 686.6 eV (SiO_xF_y), while Ge is below detection and the Si 2p oxide component stays at the native level on all samples.

A single sacrificial cure (5 min dry O_2 oxidation at 800 °C growing 2.5 nm, followed by oxide strip) recovers both axes at once (Fig. 1b,c): R_q of the CDE surface drops by 59% to 0.74 nm, the wet surface stays pristine, and the fluorine disappears below detection on every sample. PEALD SiO_2 cycle splits show identical growth on both surfaces (1.67 Å/cycle), so the electrical comparison probes the interface alone.

Because the cure erases the chemical difference, MOSCAPs (PEALD $\text{SiO}_2/\text{HfO}_2/\text{TiN}$) on four splits (dry/wet release × with/without cure) isolate the effect of the remaining roughness on D_{it} . For the uncured dry split we anticipate a mid-gap D_{it} on the order of $10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$, versus the low- 10^{11} range for the cured and wet-released splits. Measured D_{it} , V_{FB} , and hysteresis will be presented, with correlation to GAAFET devices in fabrication.

4:45pm **PCSI1-WeA2-34 Digital Etching of Single-Crystalline Silicon Fin Barriers Down to Sub-10 nm**, YU WU, University of California at Santa Barbara

A superconducting transmon qubit consists of a shunt capacitor in parallel with a nonlinear inductor, a Josephson Junction (JJ). The conventional JJ is composed of two superconducting aluminum contacts separated by thin amorphous aluminum oxide (AlO_x). It is believed that the high density of two-level system defects in or near the barrier limits the qubit performance. One promising route towards low-loss JJs is utilizing single-crystalline dielectric materials, which lack the structural disorder believed to be responsible for TLS in amorphous oxides. High-resistivity undoped float-zone Si is one of the lowest-loss dielectric materials at cryogenic temperatures and microwave frequencies. Based on first-principles calculations of Schottky barrier heights indicate that to achieve sufficient Josephson critical current density requires a Si barrier thickness in the 5~10 nm regime for Al contacts.

This work presents a fabrication process to realize sub-10 nm thick, high-aspect-ratio single-crystalline Si fins. Fins are defined on float-zone Si (110) by electron-beam lithography and anisotropic KOH etching through an LPCVD SiN_x hard mask, which also serves as the shadow mask for the subsequent superconductor angle deposition. Following the anisotropic wet etching, a digital etching process based on repeated oxidation and hydrofluoric acid etching of the resulting oxide was developed until the desired thickness is achieved. Fin thickness as thin as 6 nm has been achieved. We have investigated oxidation methods ranging from room-temperature ozone oxidation to rapid thermal annealing (RTA) oxidation at various temperatures and ambients, with liquid and vapor HF for oxide removal, using cross-sectional transmission electron microscopy to determine the thickness and roughness of the barriers. RTA oxidation provides better oxide thickness tunability, and the ramp ambient governs the thickness uniformity along the fin. In this presentation, we will discuss how the choice of oxidation and etching method affects the fin thickness and the uniformity of the barrier.

4:50pm **PCSI1-WeA2-35 Focused Helium Ion Beam Nanofabrication by Near Surface Swelling**, Sherry Mo, University of California, Berkeley

The focused helium ion beam microscope is a versatile imaging and nanofabrication instrument with sub-10 nm resolution. Subsurface damage and swelling of substrates due to helium ion implantation is generally unwanted. However, these effects can also be leveraged for specific manipulation of substrates and delicate 2D materials. To explore this, we investigate focused helium ion beam induced swelling of bulk crystalline silicon and free-standing amorphous silicon nitride membranes using various irradiation strategies. We show that the creation of near-surface voids due to helium ion implantation can be used to induce surface nanostructure and create subsurface nanochannels. Potential applications of this single-step fabrication technique include surface texturing for strain

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engineering of supported and suspended 2D materials as well as nanoimprint lithography.

4:55pm **PCSI1-WeA2-36 Accessible, Cleanroom-Free Surface Acoustic Wave Resonators**, David Shaw, Andrew Reid, Mariana Fazio, Kimia Witte, University of Strathclyde, UK

Surface Acoustic Wave (SAW) devices are a foundation for telecommunications and sensor technologies. However, commercial deployment is bottlenecked by expensive cleanroom manufacturing, requiring vacuum-based physical vapor deposition and multi-step photolithography to pattern Interdigitated Transducers (IDTs) directly onto the piezoelectric film. While solution based Chemical Bath Deposition (CBD) offers a low-cost, benchtop alternative, undoped zinc oxide (ZnO) films exhibit high n-type conductivity due to unintentional incorporation of shallow-donor impurities, primarily hydrogen. This causes the applied RF signal to dissipate as a parasitic electrical short. To overcome these limitations, we introduce a dual-strategy approach. First, copper (5 at.% Cu) is introduced into the CBD precursor solution to act as a deep acceptor, trapping the free electrons and restoring the films piezoelectric properties. Second, films are grown onto glass pre-coated with a conductive Indium Tin Oxide (ITO) underlayer to terminate electric field lines and prevent energy dispersion into the substrate. Traditional lithographic IDTs are replaced with off-the-shelf Flexible Printed Circuit Boards and are mechanically coupled to the films. Electrical and acoustic characterization validates the success of this platform. Undoped CBD films show a flat and featureless response, whereas the 5 at.% Cu-doped films exhibit a well-defined Rayleigh resonance mode at 15.4MHz. The ZnO/ITO/Glass architecture demonstrated a significantly deeper reflection magnitude and an improved electromechanical coupling coefficient compared to films grown on bare glass. 3D Laser Doppler Vibrometry (LDV) confirms the out-of-plane Rayleigh wave generation, showing a 27% increase in peak mechanical displacement (56 pm vs. 44 pm) for the ITO-supported configuration. By combining wet-chemical defect engineering, structural field confinement, and mechanical off-the-shelf components, this work establishes a fully functional, highly accessible method for rapid, low-cost SAW device manufacturing.

PCSI

Room Ballroom - Session PCSI-ThM

Semiconductor Heterostructures & Epitaxy

Moderator: Joe Falson, Caltech

8:30am **PCSI-ThM-1 Epitaxial Growth, Materials Characterization, and Detector Assessments of Quinary GaInAsSbBi**, *Rigo Carrasco, Alexander Newell, Zinah Alsaad, Julie Logan, Christian Morath, Diana Maestas*, Air Force Research Laboratory, USA; *Christopher Hains*, Aerovironment Inc, USA; *Preston Webster*, Air Force Research Laboratory, USA

INVITED

Alloying Bi in group III-V material systems has been the subject of extensive study due to the large bandgap reduction behavior per percent of Bi incorporated, and the high degree of device optimization flexibility this property affords. When alloyed with infrared materials, such as InAsSb to create InAsSbBi, a wide design space is unlocked where lattice constant and bandgap may be tuned to desired wavelengths, while maintaining a lattice-matched condition to a commercially available substrate. However, achieving proper Bi compositions in this alloy to the desired wavelength extension while maintaining smooth surface morphologies, and device-ready optoelectronic quality proved to be difficult.

Adding Ga to the mix may offer a path to mitigate these difficulties. Here, quinary GaInAsSbBi alloys are grown lattice matched on GaSb by molecular beam epitaxy. Essential and rapid growth feedback by Normarski interference contrast imaging is used to determine the ideal Bi flux condition to attain smooth surface morphologies. Fortunately, with only 0.3% Bi, ~14% Ga and corresponding As and Sb compositions that allow for a lattice-matched condition, photoluminescence extending beyond 5 μm emission, and minority carrier lifetimes $> 1 \mu\text{s}$ were realized. This motivated *nBn* device structures to be grown and fabricated into variable area single pixel device arrays. Detector dark current, and quantum efficiency are determined as a function of bias, temperature and displacement damage due to 63 MeV proton irradiation. The *nBns* are also fabricated into small format 350x256 focal plane arrays and hybridized to an analog read-out integrated circuit. This allows for direct evaluations of sensitivity, noise spectra, uniformity, operability, and radiation tolerance. A discussion on the growth feedback strategy, materials characterization results and device performance will be provided, followed by current efforts and progress.

9:00am **PCSI-ThM-7 Pressure-Dependent Photoluminescence and Strain Response of a 1.7 μm Cutoff InGaAsSb/AlGaAsSb Multi-Quantum Well**, *Meghan Verano*, New Mexico State University

The photoluminescence response of a molecular beam epitaxy-grown InGaAsSb/AlGaAsSb multi-quantum well heterostructure is investigated as a function of hydrostatic pressure up to 1.35 GPa at 10 K. Pressure-dependent photoluminescence measurements were performed using a diamond anvil cell, with pressure calibrated by ruby fluorescence. The emission peak exhibits a systematic blue shift with increasing pressure, with a measured pressure coefficient of approximately 77 meV/GPa. At the same time, the integrated photoluminescence intensity decreases with pressure, consistent with enhanced non-radiative recombination through a defect level located above the conduction-band edge at ambient pressure that becomes electronically active under compression. The strain in the quantum well is quantified using the Murnaghan equation of state, and analysis of the transition energy as a function of strain yields a hydrostatic deformation potential of approximately -4.4 eV. These measurements demonstrate the use of hydrostatic pressure as a sensitive probe of band-structure evolution, strain response, and defect-mediated recombination in quaternary III-V quantum-well heterostructures, providing insight relevant to the optimization of infrared optoelectronic materials and devices.

9:05am **PCSI-ThM-8 Probing THz-Driven Excitons in Magnetic and Conventional Semiconductors**, *Meghan Verano*, New Mexico State University

When a terahertz field is driven into a material, it is theorized that excitons in conventional semiconductors, such as gallium arsenide, will first ionize and then stabilize with increasing field strength. This adiabatic stabilization is something we aim to observe using absorption spectroscopy techniques. We first predict to see the exciton peak broaden and suppress asymmetrically as a result of the THz coupling to and disrupting the exciton. Following this broadening, the peak should again narrow, indicating an increase in exciton lifetime. The ionization rate can be extracted from fitting the Fano resonance to the absorption line shapes. In preparation for this planned THz experiment, control data has been taken on bulk and quantum well gallium arsenide using absorption spectroscopy with near infrared LED in the range of 820 - 870 nm. Nickel phosphorus trisulphide is another

material of interest. As a Mott insulator, the excitons pair in different ways than a conventional semiconductor. NiPS₃ excitons rely on the antiferromagnetic ordering of the material to survive, and this ordering is only present below 150 K. These excitons are far more robust, with a binding energy of a few hundred meV, and do not arise out of conventional band theory. We hope to use THz pump along with spectroscopy as a probe to observe magnon-exciton coupling by observing how the exciton spectrum changes under resonant pumping of magnon mode at 300 GHz in the absorption data, and phonon-exciton coupling in photoluminescence data. NiPS₃ samples have been prepared using an exfoliation and stacking technique using tape and a polymer stamp, as this Van der Waals material can be stripped down to atomically thin layers. This work is supported by NSF DMR 2333941 and NSF PREM grant DMR-2423992.

9:10am **PCSI-ThM-9 Spin-Orbit-Coupled Electronic and Vibrational Properties of ZnO/ZnS Quantum-Dot Heterostructures**, *Wisdom Benson*, Howard University

ZnO/ZnS quantum-dot heterostructures combine a polar oxide core with a wide-bandgap sulfide shell. Quantum confinement, local strain, and chemical bonding at the interface can change band-edge states and lattice vibrations. We connect Raman spectroscopy with first-principles calculations to study these coupled electronic, vibrational, dielectric, and spin-dependent effects.

We construct an isolated 2,870-atom Zn₁₃₆₆O₃₁₀S₁₁₉₄ model from a MatterSim-relaxed geometry. PBEsol/SIESTA calculations test the large heterostructure. A 42-atom Zn₁₄O₂₈ reference uses our published Quantum ESPRESSO workflow [1]: PBE+U, fully relativistic norm-conserving pseudopotentials, noncollinear spin-orbit coupling, and density-functional perturbation theory. These calculations provide band-edge orbital character, phonon modes, Raman tensors, Born effective charges, and dielectric response. Room-temperature 532 nm Raman spectra provide the experimental mode reference.

The ZnO reference has a calculated 4.54 eV HOMO-LUMO gap. Its valence edge is mainly O 2p, its conduction edge is mainly Zn 4s, and Zn 3d states lie several electronvolts below the Fermi level. Spin-orbit coupling slightly narrows the gap and lifts valence-edge degeneracies by about 0.1 eV. In the ZnO/ZnS structure, O occupies the inner region, S forms the outer shell, and Zn spans both regions. This geometry provides a direct basis for testing how interface strain and local bonding reshape band-edge and Raman-active states. The combined workflow links measured phonons to atomic structure, dielectric screening, and spin-dependent electronic behavior. These links support rational interface design for ultraviolet optoelectronics, sensing, and quantum technologies.

9:15am **PCSI-ThM-10 Sapphire Nitridation for Highly Crystalline (0002) AlN Heteroepitaxy**, *Spencer Gellerup*, Oak Ridge National Laboratory; *Matthew Brahlek, Kyle Kelley*, Oak Ridge National Laboratory

Direct nitridation of sapphire and aluminum oxide substrates via nitrogen plasma treatments is well reported for improving heteroepitaxy of AlN. In this work, plasma treatments of c-plane sapphire were conducted in-situ in a sputtering chamber directly preceding AlN deposition. Plasma treatment parameters were varied to investigate variations in resulting aluminum oxynitride formation via x-ray reflection, where x-ray diffraction was used to determine AlN crystalline texture and mosaicity. AlN (0002) rocking curve full-width-half max of ~0.1° was measured for optimal sapphire plasma treatments. A narrow processing window is reported to maintain crystalline registry with the sapphire substrate, without growing too thick and rough leading to disordered AlN films. Transmission electron microscopy interrogated the thickness, crystallinity, and stoichiometry via electron energy loss spectroscopy (EELS) of the aluminum oxynitride buffer layer. Improving AlN quality through the use of nitriding sapphire with CMOS compatible fabrication will enhance device performance and templating with other materials.

9:20am **PCSI-ThM-11 TiZrN-based Coatings for Dry Machining Deposited by Dual-beam EB-PVD**, *Glenn Cassar, Andre Giordimaina, Kieran Axisa*, University of Malta

TiZrN-based hard coatings are attractive candidates for dry machining applications, but their deposition via electron-beam physical vapor deposition is typically limited by markedly different evaporation rates between Ti and Zr. In this study, TiZrN-based coatings were developed on AISI H13 (DIN 1.2344) steel substrates using a plasma-assisted dual-beam EB-PVD process. Such coatings were investigated for the long-term objective of enabling multifunctional Ti-Zr coating systems, such as TiZrCrN, but initial trials showed preferential Ti evaporation from the melt pool,

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generating a Ti-rich vapor flux and restricting Zr incorporation. To avoid Zr-depleted coatings, Ti-Zr targets with varied Ti:Zr ratios were investigated to compensate for the differential evaporation and to achieve compositionally controlled TiZrN-based coatings. The deposited coatings were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX) nanoindentation and pin-on-disk tribology, with emphasis on the correlation between composition, microstructure, mechanical properties, and wear behavior relevant to dry-machining conditions. By treating source chemistry as an active process-control variable, the study aims at providing an EB route towards compositionally controlled TiZrN-based coatings for lubricant-free machining.

11:00am **PCSI-ThM-31 Closing Remarks**

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