

## Quantum Science and Technology Mini-Symposium Room 208 W - Session QS1-MoM

### Qubit Modalities for Quantum Computing

**Moderators:** Ekta Bhatia, NY CREATES, Drew Rebar, Pacific Northwest National Laboratory

8:15am **QS1-MoM-1 Strongly Anharmonic Gatemon Devices on Proximitized InAs 2DEG**, *Shukai Liu*<sup>1</sup>, University of Maryland, College Park; *Arunav Bordoloi*, *Jacob Issokson*, *Ido Levy*, New York University; *Kasra Sardashti*, University of Maryland College Park; *Javad Shabani*, New York University; *Vladimir Manucharyan*, EPFL, Switzerland

Gatemon qubits represent an all-electric variant of the conventional transmon, where local electrically gated superconductor-semiconductor hybrid Josephson junctions (JJs) are employed for qubit operations. Gatemon qubits, made of transparent super-semi Josephson junctions, typically have even weaker anharmonicity than the opaque AlO<sub>x</sub>-junction transmons. However, flux-frustrated gatemons can acquire a much stronger anharmonicity, originating from the interference of the higher-order harmonics of the supercurrent. Here, we investigate this effect of enhanced anharmonicity in split-junction gatemon devices based on a proximitized InAs quantum well. We find that anharmonicity over 100% can be routinely achieved at the half-integer flux sweet-spot without any need for electrical gating or excessive sensitivity to the offset charge noise. We verified that such “gateless gatemon” qubits can be driven with Rabi frequencies more than 100 MHz, enabling gate operations much faster than what is possible with traditional gatemons and transmons. Furthermore, by analyzing a relatively high-resolution spectroscopy of the device transitions as a function of flux, we were able to extract fine details of the current-phase relation, to which transport measurements would hardly be sensitive. The strong anharmonicity of our gateless gatemons, along with their bare-bones design, can prove to be a precious resource that transparent super-semi junctions bring to quantum information processing.

8:30am **QS1-MoM-2 Quantum Keynote Lecture: Evolution of IBM Quantum Processors Towards Advantage and Quantum Error Correction**, *David McKay*<sup>2</sup>, *Jerry Chow*, IBM Quantum **INVITED**

To achieve the ultimate goal of quantum computing – fault tolerance – we need to push performance to the limit, in particular quality and scale. IBM has been a leader in both; in 2021 we debuted the 127-qubit fixed-frequency fixed-coupling Eagle processor. The Eagle processor had unparalleled stability and coherence but was limited by crosstalk in the fixed-coupling architecture. This limitation drove the development and release of the 156 qubit Heron processor in 2023, utilizing a fixed-frequency tunable-coupling architecture. When benchmarked at scale, using error per layered gate (EPLG) at 100 qubits [1], the Heron is up to a 10x improvement over the Eagle. In this talk, I will discuss some of the technological improvements required to build these devices, expand on measuring quality at scale using EPLG [1] and Cliffordization [2], and introduce our next device scheduled for later this year, the 120 qubit Nighthawk. The Nighthawk processor is an evolution of the Heron with grid connectivity to accelerate to the era of quantum advantage [3]. Finally, I will discuss our quantum error correction roadmap based on a low-density parity-check (LDPC) code [4]. This code improves encoding rate by requiring long range checks. Implementing the required long-range couplers is the next node of our innovation roadmap and will be implemented in a future exploratory processor “Loon”.

[1] arXiv:2408.07677 [2] arXiv:2503.05943 [3] arXiv:2506.20658 [4] arXiv:2506.03094

9:15am **QS1-MoM-5 Stable CNOT-Gate on Inductively-Coupled Fluxoniums with Over 99.9% Fidelity I**, *Wei-Ju Lin*, University of Maryland College Park, Taiwan; *Hyunheung Cho*, University of Maryland College Park, Republic of Korea; *Yinqi Chen*, Louisiana State University, China; *Kasra Sardashti*, Laboratory for Physical Sciences; *Maxim Vavilov*, University of Wisconsin - Madison; *Chen Wang*, University of Massachusetts - Amherst; *Vladimir Manucharyan*, EPFL, Switzerland

In this part of the talk, we report a detailed characterization of two inductively-coupled superconducting fluxonium qubits [1] for implementing high-fidelity cross-resonance gates [2]. Our circuit is notable because it behaves very closely to the case of two transversely coupled spin- $\frac{1}{2}$  systems.

In particular, the generally unwanted static ZZ-term resulting from the non-computational transitions is nearly absent, even with a strong qubit-qubit hybridization. Spectroscopy of the non-computational transitions reveals a spurious  $\frac{1}{2}LC\phi$ -mode arising from the combination of the coupling inductance and the capacitive links between the terminals of the two-qubit circuit. Such a mode has a minor effect on the present device, but it must be carefully considered for optimizing future multi-qubit designs.

[1] Lin, Wei-Ju, et al. "Verifying the analogy between transversely coupled spin-1/2 systems and inductively-coupled fluxoniums." *New Journal of Physics* 27.3 (2025): 033012.

[2] Lin, Wei-Ju, et al. "24 Days-Stable CNOT Gate on Fluxonium Qubits with Over 99.9% Fidelity." *PRX Quantum* 6.1 (2025): 010349.

9:30am **QS1-MoM-6 Stable CNOT-Gate on Inductively-coupled Fluxoniums with over 99.9% Fidelity II**, *Wei-Ju Lin*, *Hyunheung Cho*, University of Maryland, College Park; *Yinqi Chen*, University of Wisconsin - Madison; *Kasra Sardashti*, University of Maryland, College Park; *Maxim G. Vavilov*, University of Wisconsin - Madison; *Chen Wang*, University of Massachusetts, Amherst; *Vladimir E. Manucharyan*, EPFL, Switzerland

In this part of the talk, we discuss the realization of a 60 ns direct CNOT gate on two inductively-coupled fluxonium qubits over 99.9% fidelity [1]. Fluxonium qubit is a promising elementary building block for quantum information processing due to its long coherence time combined with a strong anharmonicity. In this paper, we realize a 60 ns direct CNOT-gate on two inductively-coupled fluxoniums, which behave almost exactly as a pair of transversely-coupled spin- $\frac{1}{2}$  systems [2]. The CNOT-gate fidelity, estimated using randomized benchmarking, was as high as 99.94%. Furthermore, the fidelity remains above 99.9% for 24 days without any recalibration between measurements. Compared with the 99.96% fidelity of a 60 ns identity gate, our data brings the investigation of the non-decoherence-related errors during logical operations down to  $2 \times 10^{-4}$ . The present result adds a simple and robust two-qubit gate into the still relatively small family of the “beyond three nines” gates on superconducting qubits.

[1] Lin, Wei-Ju, et al. "24 days-stable CNOT-gate on fluxonium qubits with over 99.9% fidelity." *arXiv preprint arXiv:2407.15783* (2024).

[2] Lin, Wei-Ju, et al. "Verifying the analogy between transversely coupled spin-1/2 systems and inductively-coupled fluxoniums." *arXiv preprint arXiv:2407.15450* (2024).

9:45am **QS1-MoM-7 Silicon-Based Quantum Processors**, *Jason Petta*, University of California at Los Angeles **INVITED**

Of all of the qubit modalities being investigated, semiconductor spin qubits most closely resemble conventional transistors, which can be fabricated at scale with  $\sim 100$  billion transistors on a chip. It is therefore important to pursue long-term approaches to fault-tolerant quantum computing with spin qubits. I will give an update on recent progress, including high-fidelity multi-qubit control [1,2], long-range spin-spin coupling [3,4], and two-dimensional spin qubit arrays [5,6].

### References

- [1] A Mills *et al.*, Phys. Rev. Applied **18**, 064028 (2022).
- [2] A. Mills *et al.*, Sci. Adv. **8**, eabn5130 (2022).
- [3] F. Borjans *et al.*, Nature **577**, 195 (2020).
- [4] X. Zhang *et al.*, Phys. Rev. Applied **21**, 014019 (2024).
- [5] W. Ha *et al.*, Nano Lett. **22**, 1443 (2022).
- [6] E. Acuna *et al.*, Phys. Rev. Applied **22**, 044057 (2024).

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<sup>1</sup> JVST Highlighted Talk

<sup>2</sup> Quantum Keynote Lecture

## Quantum Science and Technology Mini-Symposium

### Room 208 W - Session QS2-MoM

#### Systems, Devices, and Manufacturing Technologies for Quantum Technology

**Moderator: Aranya Goswami**, Massachusetts Institute of Technology

##### 10:30am QS2-MoM-10 Superconducting Qubits at MIT Lincoln Laboratory, **Mollie Schwartz**, MIT Lincoln Laboratory **INVITED**

Superconducting qubits are leading candidates in the race to build a quantum computer capable of realizing computations beyond the reach of modern supercomputers. Within this modality, the ability to robustly and reliably fabricate high-quality, quantum-compatible circuits is critical both for fundamental research efforts and for more complex and capable quantum processors. MIT Lincoln Laboratory has worked over the course of two decades to establish, and continually expand and improve, superconducting qubit fabrication capabilities. Recently, we have piloted a superconducting foundry model to enable the US quantum research and development community to leverage the most robust and reliable of these capabilities in order to accelerate research progress. This presentation will provide an overview of superconducting qubit fabrication at MIT Lincoln Laboratory, describe its transition from 50 mm prototyping tools to 200 mm fabrication to support an expanded user base, and provide perspectives on how to support and enable the broader quantum research community as the variety and complexity of questions at the research frontier continues to expand.

##### 11:00am QS2-MoM-12 Voltage Tunable MBE-grown Ge/SiGe Josephson Junctions for Gateable Qubits, **Joshua Thompson**, **Jason Dong**, **Junior Langa**, Laboratory for Physical Sciences; **Brycelynn Bailey**, University of Arkansas; **Chomani Gaspe**, **Ris Card**, Laboratory for Physical Sciences; **Shiva Davari**, **Mariam Afrose**, University of Arkansas; **Thomas Hazard**, **Kyle Serniak**, MIT Lincoln Laboratory; **Kasra Sardashti**, Laboratory for Physical Sciences; **Hugh Churchill**, University of Arkansas; **Christopher Richardson**, Laboratory for Physical Sciences

Voltage tunable Josephson junctions (JJs) based on planar semiconductor quantum wells have potential to realize voltage tunable qubits fabricated at scale. Josephson junctions are fabricated from undoped Germanium quantum wells (Ge-QWs), grown by Molecular Beam Epitaxy (MBE), with carrier mobility greater than  $40,000 \text{ cm}^2/\text{Vs}$  and hole density less than  $1 \times 10^{12} \text{ cm}^{-2}$ . These junctions use epitaxial aluminum to make transparent contact to the Ge-QW and a mesa structure that is  $2.5\text{-}\mu\text{m}$  tall with only the JJ on top, minimizes microwave loss from epitaxial layers, which is critical for superconducting qubits. This presentation will demonstrate gate tunable critical currents and discuss the characterization of MBE-grown Ge JJs along with the path toward integrating these JJs into gateable qubits.

##### 11:15am QS2-MoM-13 Development of Ge/SiGe Semiconducting Quantum Dot Devices for Hole-Based Spin Qubits, **Giovanni Franco-Rivera**, **Jason Dong**, University of Maryland College Park; **Alan Kramer**, Laboratory for Physical Sciences; **Kasra Sardashti**, University of Maryland College Park; **Robert Butera**, Laboratory for Physical Sciences

Confining few electrons in silicon-based heterostructures via lithographically-defined, gated on-chip quantum dots (QD) enables the manipulation of the spin degree of freedom for quantum information processing. In recent years, the hole-based QDs based on strained Ge/SiGe semiconducting quantum wells have rapidly advanced as a compelling platform for spin qubits [1]. Some of the appealing features of the Ge-based spin qubits are their coherent properties achievable by solid-state all-electrical control readout enabled by their intrinsic spin-orbit interaction [2], and their prospects of scalability resulting from long-range coupling via superconducting circuits [3]. From a fabrication standpoint, two key components for the formation of the Ge-QDs is the electrical contacts to the Ge-well and the gate dielectric interface quality over the active dot area. On the aforementioned aspect, we explore the use of metallic germano-silicide contacts to the Ge quantum well due to their lower temperature requirements for the fabrication and ability to be proximitized to the quantum dot active area avoiding structural damages caused by a high fluence ion implantation. We estimate the contact resistance via low temperature transport measurements on gated transfer line method devices (TLMs) with contacts formed by platinum germano-silicides (Pt-Ge-Si). On the later aspect, the gate dielectric interface, we focus on optimizing the quality of the ALD-grown  $\text{Al}_2\text{O}_3/\text{SiGe}$  interfaces. We present the results from a series of X-ray photoemission spectroscopy (XPS) measurements on the  $\text{Al}_2\text{O}_3/\text{SiGe}$  and  $\text{Al}_2\text{O}_3/\text{Pt-Ge-Si}$  interfaces. Our XPS data points to the presence of unwanted Ge in the dielectric interface layer presenting a

medium for charge traps that contribute a significant source of charge noise in the device. Lastly, we present methods to mitigate the Ge presence in the gate stack and near the  $\text{Al}_2\text{O}_3/\text{Pt-Ge-Si}$  interface.

#### References:

[1] Scappucci, G., Kloeffer, C., Zwanenburg, F.A. et al. The germanium quantum information route. *Nat Rev Mater* 6, 926–943 (2021).

[2] Hendrickx, N.W., Massai, L., Mergenthaler, M. et al. Sweet-spot operation of a germanium hole spin qubit with highly anisotropic noise sensitivity. *Nat. Mater.* **23**, 920–927 (2024).

[3] Sagi, O., Crippa, A., Valentini, M. et al. A gate tunable transmon qubit in planar Ge. *Nat Commun* 15, 6400 (2024).

11:30am QS2-MoM-14 Post-processing of Josephson Junctions for Precision Tuning of Qubit Frequencies, **David P. Pappas**, **X Wang**, **Joel Howard**, **Greg Stiehl**, **Cameron Kopas**, **Stefano Poletto**, **Xian Wu**, **Mark Field**, **Nicholas Sharac**, **Christopher Eckberg**, **Hilal Cansizoglu**, **Raja Katta**, **Josh Mutus**, **Andrew Bestwick**, **Kameshwar Yadavalli**, Rigetti Computing; **Jinsu Oh**, Ames Laboratory; **Lin Zhou**, **Matthew Kramer**, Ames Laboratory **INVITED**

Thin layers of thermal aluminum oxide are the dominant material for making Josephson tunnel-junctions (JJs). These JJs are the key component for qubits in most superconducting implementations of quantum computing. It has become clear that it is necessary to address the issue of JJ homogeneity in order to more precisely tune the qubit frequencies. Work towards this using the newly developed alternating-bias assisted annealing (ABAA) technique will be discussed. ABAA illuminates a promising path towards precision tuning of qubit frequency post-processing while attaining higher coherence due to an apparent reduction in junction loss. Here, we demonstrate precision tuning of the qubits by performing ABAA at room temperature using commercially available test equipment and characterizing the impact of junction relaxation and aging on the resistance spread after tuning. A study of the structural properties of the material using transmission electron microscopy will be given with some thoughts of what the driving mechanism for ABAA is at the atomic scale.

## Quantum Science and Technology Mini-Symposium Room 208 W - Session QS1-MoA

### Advanced Materials for Quantum Information Science

**Moderators:** *Kasra Sardashti*, University of Maryland College Park; *David Pappas*, Rigetti Computing

#### 1:30pm QS1-MoA-1 Superconductor-Semiconductor Epitaxy in Hyperdoped Germanium, *Javad Shabani*, NYU **INVITED**

Introducing superconductivity into group IV elements by doping has long promised a pathway to introduce quantum functionalities into well-established semiconductor technologies. The non-equilibrium hyperdoping of group III atoms into Si or Ge has successfully shown superconductivity can be achieved, however, the origin of superconductivity has been obscured by structural disorder and dopant clustering. Here, we report the epitaxial growth of hyperdoped Ga:Ge films by molecular beam epitaxy with extreme hole concentrations  $10^{21}\text{cm}^{-3}$ , that yield superconductivity with a critical temperature of  $T_c = 3.5\text{K}$ . Our findings, corroborated by first-principles calculations, suggest that the structural order of Ga dopants creates a narrow band for the emergence of superconductivity in Ge, establishing hyperdoped Ga:Ge as a low-disorder, epitaxial superconductor-semiconductor platform. This platform opens up a new path for integration of superconductivity for cryogenic and quantum applications in group IV.

#### 2:00pm QS1-MoA-3 Molecular Beam Epitaxy of Germanium Quantum Wells with Epitaxial Aluminum, *Jason Dong*, *Joshua Thompson*, *Chomani Gaspe*, *Riis Card*, *Kasra Sardashti*, Laboratory for Physical Sciences; *Shiva Davari Dolatabadi*, *Hugh Churchill*, University of Arkansas; *Kyle Serniak*, *Thomas Hazard*, MIT Lincoln Laboratory; *Christopher Richardson*, Laboratory for Physical Sciences

Voltage tunable Josephson junctions (JJs) are an alternative route towards tuning the critical current of JJs in quantum circuits to enable new functionalities, and replace the current carrying flux lines and squids that are currently used. Germanium JJs implemented on float-zone silicon substrates allow for scalable integration with low-loss superconducting circuit elements, and enable a gate tunable transmon with longer coherence times. Here, Ge quantum wells (QW) with epitaxial aluminum contacts are grown by molecular beam epitaxy.

Strained Ge-QWs are grown on  $\text{Si}_{0.2}\text{Ge}_{0.8}$  virtual substrates. The  $\text{Si}_{0.2}\text{Ge}_{0.8}$  virtual substrates are grown with a reverse graded buffer layer on float zone silicon. Epitaxial aluminum is grown *in situ* on the Ge quantum wells to create high-transparency superconducting contacts that proximitize the underlying Ge-QWs. From low-temperature magneto-transport measurements, a 2 K mobility exceeding  $45,000\text{ cm}^2/\text{Vs}$  is observed for samples with a 22-nm deep QW. The effect of growth conditions on the structural quality and low-temperature mobility will be discussed. The structural quality of the samples is investigated with X-ray diffraction, atomic force microscopy, and defect selective etching. Reverse graded buffer layers with the thickness exceeding  $1.5\text{ }\mu\text{m}$  are found to be required to eliminate most structural defects. The limiting scattering mechanisms are identified from analysis of the carrier density dependence of the mobility and potential routes towards improving the mobility will be discussed.

#### 2:15pm QS1-MoA-4 Epitaxy of Superconducting Germanium Thin Films for Integrated Quantum Electronics, *Patrick Strohbeen*<sup>1</sup>, New York University; *Julian Steele*, *Ardeshtir Baktash*, university of queensland, Australia; *Alisa Danilenko*, new york university; *Axel Leblanc*, *Jechiel van Dijk*, New York University; *Yi-Hsun Chen*, *Lianzhou Wang*, university of queensland, Australia; *Salva Salmani-Rezaie*, Ohio State University; *Eugene Demler*, ETH Zurich, Switzerland; *Peter Jacobson*, university of queensland, Australia; *Javad Shabani*, New York University

Superconducting group IV materials are highly promising for quantum information due to the homoepitaxial alignment with the underlying substrate, reducing material disorder at the film/substrate interface. Furthermore, increasing interest in germanium systems for both spin qubits, gate-tunable superconducting qubits, and topological phases has put a spotlight on the necessity for thin film superconductors that readily interface with group IV systems. However, the hyperdoped phase is thought to require dopant incorporation above typical thermodynamical solubility limits and thus most efforts have been focused on non-equilibrium techniques. Very recent work has shown that superconductivity is observed in Ga-doped germanium system using molecular beam epitaxy. In this talk

we will present an expanded study towards illuminating the atomic fine structure of superconducting germanium thin films grown via MBE. We observe that our superconducting MBE-grown films exhibit well-dispersed Ga-dopants throughout the film as substitutional defects via synchrotron-based X-ray scattering and absorption experiments. Cross-sectional electron microscopy imaging shows the homoepitaxial interface between the Ge substrate and the superconducting Ge film is well-defined, the films are of high crystalline quality, and no Ga clustering is found. Band structure calculations further suggest that the observed crystal structure induced a narrow-band state at the R-point in the Brillouin Zone, posing a new possible mechanism for the observed superconducting state.

#### 2:30pm QS1-MoA-5 Growth and Characterization of Thin-Film A15 Nb-Al Intermetallics for Superconducting Quantum Electronics, *Joseph Falvo*<sup>2</sup>, University of Maryland College Park; *Elizabeth Henry*, Clemson University; *Ashish Alexander*, University of Maryland; *Hussein Hijazi*, Rutgers University; *Ivan Lainez*, University of Maryland; *Leonard Feldman*, Rutgers University; *Kasra Sardashti*, Laboratory for Physical Sciences

As superconducting qubit technology progresses, there is an increasing demand for materials with high critical temperatures and critical magnetic fields to allow for devices to be more robust against external excitations. A15 intermetallic compounds, a family of superconductors explored in the 1950's through the 1970's, provide one potential avenue to such high critical values. In this work, we synthesize Nb<sub>3</sub>Al, one of many A15 compounds, as a thin film by co-sputtering from elemental targets, followed by a rapid thermal annealing procedure. We confirm the realization of the desired ratio and crystal structure within our films by Rutherford backscattering (RBS) and X-ray diffractometry, respectively. For films with thickness close to 200 nm, we achieve thin films with  $T_c$  greater than 16 Kelvin and zero-temperature critical fields greater than 30 T. Additionally, we report single-photon microwave quality factors of  $1.9 \times 10^5$  and estimates for kinetic inductance similar to NbN at comparable thickness.

#### 2:45pm QS1-MoA-6 High Purity Physical Vapor Deposition CaO Thin Films for Quantum Information Science, *Jake DeChiara*, *Saeed Almishal*, Pennsylvania State University; *Jon-Paul Maria*, Pennsylvania State University

CaO has generated substantial interest in the quantum informatics community as a novel solid state Qubit host. In this work we aim to experimentally verify the existence of Schottky defects with rare earth and bismuth interstitials in a high purity CaO thin film host grown on R-plane Sapphire. We study reactive RF sputter and pulsed laser deposition techniques utilizing metallic calcium and  $\text{Ca}(\text{OH})_2$  targets. X-ray fluorescence reveals that metallic calcium targets contain substantial chlorine impurities, which adversely affects CaO film growth via sputtering. We demonstrate  $\text{Ca}(\text{OH})_2$  as an intriguing candidate as a calcium source for physical vapor deposition due to its availability in high (99.999%) purity and relatively low cost. We utilize a hydrothermal sintering method to attain target density above 95 % while maintaining high chemical purity. All CaO thin films grown were found to achieve single orientation in the (0 0 2) direction, as verified via X-Ray diffraction. Film thickness evaluated by X-Ray reflectivity measurements revealed a faster deposition rate from the metallic calcium target compared to the  $\text{Ca}(\text{OH})_2$  target during sputter deposition. Deposition growth rates achieved from the  $\text{Ca}(\text{OH})_2$  targets were highly linear and suggest high target stability and reliability. CaO films grown by pulsed laser deposition attained high crystallinity, relatively fast deposition rates, and single orientation. We have identified a wide range of methods in the physical vapour deposition processing space which permit further investigation into the defect structure of doped CaO thin films.

#### 3:00pm QS1-MoA-7 Extending the Specific Resistance of Alox Thin Films by Tuning Plasma Oxidation Time for Qis Devices, *Runze Li*, University of Maryland, College Park; *Joshua Pomeroy*, National Institute of Standards and Technology

We are extending the range of the specific resistance for our Plasma-Alox tunnel barriers based on adjusting the oxidation time to reach  $1\text{ G}\Omega \cdot \mu\text{m}^2$ . Device instabilities like charge drift and loss tangent are persistent problems for QIS devices like Josephson junctions that significantly reduce the device stability or shorten the decoherence time. By using plasma oxidation and *in situ* techniques for device fabrication, we have greatly increased the stability of our AlOx tunnel junctions. We believed that generating oxygen atoms in the plasma results in higher reactivity than the

<sup>1</sup> JVST Highlighted Talk

<sup>2</sup> JVST Highlighted Talk

oxygen molecules present in natural oxidation. Hence, a denser and less defective aluminum oxide is formed through plasma oxidation. As a result, we have observed a  $\approx 50$  times increase in the plasma-AlOx based Single Electron Transistors (SETs) compared to naturally oxidized AlOx based SETs (Zimmerman, 2008). We will report on the fabrication and characterization of our plasma-AlOx thin film for thickness and composition change v.s. oxidation time.

## 3:15pm QS1-MoA-8 Epitaxial Control of Magnetism and Superconductivity in Quantum Materials, *Matthew Brahlek*, Oak Ridge National Laboratory

INVITED

Understanding and designing functional quantum phenomena presents significant challenges due to the complexity of integrating structurally dissimilar materials and managing intertwined factors such as valence, spin, orbital, and structural degrees of freedom. In this talk, I will highlight recent discoveries that demonstrate how novel phenomena can emerge at the interfaces of materials synthesized as high-quality thin films via molecular beam epitaxy. I will also discuss how advancements in x-ray techniques have provided new insights into the origins of these properties. These findings include emergent and tunable ferromagnetism [1], interfacially enhanced superconductivity [2–3], and the proposed emergence of altermagnetism [4]. A key takeaway is that these breakthroughs are made possible by the tight integration of material synthesis with structural and spectroscopic x-ray-based probes. This combined approach is essential for unraveling the origins of functional quantum phenomena and exploring how these exotic phases can be controlled—potentially paving the way for next-generation microelectronic devices.

[1] M. Brahlek *et al.*, Nano Letters, 23, 7279-7287 (2023); 10.1021/acs.nanolett.3c01065

[2] R. G. Moore *et al.*, Advanced Materials, 35, 2210940 (2023); 10.1002/adma.202210940

[3] A.-H. Chen *et al.*, Advanced Materials, 202401809 (2024); 10.1002/adma.202401809

[4] M. Chilcote *et al.*, Advanced Functional Materials, 2405829 (2024); 10.1002/adfm.202405829

## Quantum Science and Technology Mini-Symposium Room 208 W - Session QS2-MoA

### Surface Engineering for Quantum Applications

**Moderators:** *Dave Pappas*, Rigetti Computing, *Drew Rebar*, Pacific Northwest National Laboratory

## 4:00pm QS2-MoA-11 Towards Reducing Dielectric Loss from Josephson Junctions in Superconducting Qubits, *Aranya Goswami*, *Hung-Yu Tsao*, *Chia-Chin Tsai*, *Kyle Serniak*, *Jeffrey A. Grover*, *William D. Oliver*, Massachusetts Institute of Technology

Superconducting qubits are a promising platform to build large-scale quantum computers. However, material imperfections and defects induced by various nanofabrication processes result in the formation of two-level systems (TLSs). TLSs reduce coherence times and increase temporal fluctuations, making qubits harder to operate in a system. One of the major sources of such TLSs has been observed to arise from the dielectric inside the Josephson junctions as well as residues/surface dielectric oxide on the metal surrounding the junction. Here we study this in two parts.

First, we look at the impact of oxidation parameters on the behavior of the Al/AlOx/Al Josephson junctions. We specifically study the effects of oxidation pressure and flow during the AlOx formation on the coherence times of the qubits. Using this process, we attempt to identify oxidation conditions that improve coherence and reproducibility for wafer-scale qubit processing.

In the second part of this talk, we present a wafer-scale inorganic stencil-mask based technique to fabricate the Josephson junctions for superconducting qubits. Using this platform, we compare the effects of a resist-free vs resist-based processes on the coherence times of transmon qubits.

## 4:15pm QS2-MoA-12 HF Induced Degradation in High-Purity, Epitaxial Thin Film Niobium, *Haozhi Wang*, University of Maryland, College Park; *Tathagata Banerjee*, Cornell University; *Thomas Farinha*, University of Maryland, College Park; *Aubrey Hanbicki*, Laboratory for Physical Sciences; *Valla Fatemi*, Cornell University; *Benjamin Palmer*, *Christopher Richardson*, Laboratory for Physical Sciences

As a high-gap superconductor, Niobium (Nb) is a natural choice for making supercomputing qubits that can be operated at elevated temperatures. Nowadays, HF based acid cleans have become a regular processing step to remove native oxide and boost device performance. However, one impurity that severely degrades the superconducting properties of Nb is hydrogen (H). Without a protective NbOx layer, Nb can absorb H, and at a large enough H concentration, niobium hydrides (NbH) precipitate. In this talk, we present the impact of HF-based acid cleans on an ultrahigh purity single crystal Nb film grown on sapphire with  $T_c = 9.23$  K, RRR = 40, and resonators with single-photon quality factors more than  $10E6$ . Depending on the exposure to HF-based solutions, a degradation of the both dc and rf performances are observed. Unique crystallite defects with heights of 50 nm and 3-fold symmetry, which we identify as hydrides, are also observed. The contaminated Nb material is further characterized using x-ray diffraction, x-ray photoelectron spectroscopy, and Raman spectroscopy.

## 4:30pm QS2-MoA-13 Reducing Losses in Transmon Qubits Using Fluorine-Based Etches, *Michael Gingras*, *Bethany Niedzielski*, *Felipe Contipelli*, *Ali Sabbah*, *Kate Azar*, *Greg Calusine*, *Cyrus Hirjibehedin*, *David Kim*, *Jeff Knecht*, *Christopher O'Connell*, *Alexander Melville*, *Hannah Stickler*, *Mollie Schwartz*, *Jonilyn Yoder*, MIT Lincoln Laboratory; *William Oliver*, MIT; *Kyle Serniak*, MIT Lincoln Laboratory

Superconducting qubits have developed from proof-of principle single-bit demonstrations to mature deployments of many-qubit quantum processors. Reducing materials- and processing-induced decoherence in superconducting qubit circuits is critical to further the development of large-scale quantum architectures. In this talk we discuss the results of applying selective fluorine-based etches, targeting lossy silicon oxides, in close proximity to sensitive aluminum circuit elements such as Josephson Junctions, resonators and crossover tethers. These fabrication improvements can be implemented with little to no damage to existing structures. The impact that these have on transmon qubit coherence will be discussed.

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## 4:45pm QS2-MoA-14 Understanding and Mitigating Coherence and Frequency Fluctuations in Superconducting Transmon Qubits, *Tanay Roy*, *Xinyuan You*, *Bektur Abdisatarov*, *Daniel Bafia*, *Mustafa Bal*, *David van Zanten*, *Alexander Romanenko*, *Anna Grassellino*, Fermi Lab

Transmon qubits are a cornerstone of superconducting quantum computing platforms. However, their frequency and coherence properties exhibit temporal fluctuations, leading to performance degradation in quantum processors over time. A common mitigation approach involves frequent recalibration, which, while effective, results in increased system downtime. Enhancing the long-term stability of transmon qubits is therefore critical for scalable and reliable quantum computing. In this study, we develop novel techniques for understanding the underlying mechanisms driving frequency and coherence fluctuations in fixed-frequency transmon qubits. We further explore strategies to mitigate these instabilities, aiming to improve overall system robustness. Our findings provide insights into optimizing superconducting quantum hardware for practical applications.

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## 5:00pm QS2-MoA-15 Platinum Encapsulation of Niobium and Tantalum Thin Films for Low-Loss Superconducting Qubit Interfaces, *Ananya Chattaraj*, Brookhaven National Laboratory

Superconducting qubits are fundamental components of many quantum computing platforms, yet their scalability is fundamentally limited by decoherence mechanisms arising from environmental disturbances. A critical challenge lies in mitigating dielectric losses associated with surface oxides on superconducting films, which contribute to two-level system (TLS) noise—a dominant decoherence source. Niobium (Nb) and tantalum (Ta)

are key superconducting materials used in transmon qubits, but native oxide layers formed during fabrication degrade coherence times. Recent advances have pushed tantalum-based qubits to coherence times approaching 0.3 ms; however, further improvements require refined control over interfacial chemistry and oxide suppression. In this study, we explore platinum (Pt) capping layers as a materials-engineering strategy to reduce oxide formation and dielectric loss on Nb and Ta thin films. The films were deposited via optimized sputtering under oxygen-free conditions to ensure high purity and preserve superconducting properties. Initial laboratory characterization by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) confirmed phase purity and reduced oxidation. High-quality films were further analyzed with advanced synchrotron-based techniques, including grazing-incidence extended X-ray absorption fine structure (GI-EXAFS) and variable photon energy hard X-ray photoelectron spectroscopy (HAXPES). These element-specific, depth-resolved methods enabled detailed probing of the Pt/Nb and Pt/Ta interfacial structures, revealing the atomic-scale environment, oxidation states, and any potential alloying or interdiffusion effects that can influence qubit performance. Transport measurements verified that Pt encapsulation maintained the superconducting transition temperature ( $T_c$ ) of Nb films near 9 K, demonstrating the Pt layer's efficacy as a protective barrier without compromising superconductivity. Comparative analyses between Pt/Nb and Pt/Ta interfaces highlighted differences in oxidation behavior and structural stability, offering critical insights for material selection and interface design in qubit fabrication. This work advances the understanding of interfacial engineering approaches in quantum device materials and provides a pathway toward scalable, low-loss superconducting qubit architectures.

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## Electronic Materials and Photonics

Room 207 A W - Session EM1+AP+CPS+MS+PS+QS+SM+TF-TuM

### Emerging Frontiers in Quantum Materials and Devices

Moderator: Mollie Schwartz, MIT Lincoln Laboratory

8:30am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-3 Rapid, Atomic-Scale Smoothing of GaSb(111)A Surfaces During Molecular Beam Epitaxy, James Rushing, Paul Simmonds, Tufts University**

InAs/Ga(In)Sb quantum wells (QWs) with a broken gap band alignment can behave as a quantum spin hall insulator (QSHI) with an insulating bulk and topologically protected helical edge states [1-2]. QSHIs could be a key component in spintronic and topological quantum computing applications [2-3]. Producing a topological phase transition in InAs/Ga(In)Sb QWs requires precise control of QW thickness, composition and quality, particularly at the heterointerfaces. Additionally, our calculations suggest QWs grown on (111) surfaces could provide benefits over (001) due to the higher symmetry and out-of-plane polarization effects of this surface.

While exploring the MBE growth of InAs/Ga(In)Sb QW heterostructures on GaSb(111)A, we discovered an exciting and confounding phenomenon that seems to be unique to crystal growth on III-Sb(111)A surfaces. Ga(In)Sb(111)A frequently exhibits an extremely rough morphology characterized by pyramidal peaks covering the entire surface. We show that rough III-Sb surfaces (pyramidal features >70nm in height; rms roughness >10nm), can be smoothed to atomically flat surfaces (<3nm height features; <0.5nm rms roughness) in a matter of seconds by exposing them to an arsenic over-pressure. We first observed this phenomenon when rough GaInSb(111)A surfaces became atomically flat after capping with just 8nm of InAs. After reducing the thickness of this InAs layer to a single monolayer and still observing the same surface smoothing effect, we found that we could achieve almost identical results by simply exposing the rough GaSb(111)A to an arsenic flux. These results suggest that arsenic is the primary mover in these profound morphological changes. Our recent results show that the smoothing can be accomplished with As<sub>4</sub> or As<sub>2</sub>, and with a wide range of arsenic beam equivalent pressures, from 5x10<sup>-7</sup> to 1x10<sup>-5</sup> Torr.

We will describe our efforts to gain control and understanding of this phenomenon through the modulation of arsenic exposure time, flux, and terminating III-Sb material. This powerful new MBE technique will allow us to reliably achieve smooth heterointerfaces in (111)-oriented InAs/Ga(In)Sb QWs for novel, high-quality QSHIs. More broadly, we believe that this approach will enable the growth of a wide array of III-Sb-based nanostructures on (111)A surfaces for other electronic and photonic applications.

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8:45am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-4 Benchmarking Different NbTiN Sputtering Methods for 300 nm CMOS-compatible Superconducting Digital Circuits, Adham Elshaer<sup>1</sup>, Jean-Philippe Soulié, Daniel Perez Lozano, Gilles Delie, Ankit Pokhrel, Benjamin Huet, IMEC Belgium; Margriet J. Van Bael, KU Leuven and Imec, Belgium; Daan Buseyne, KU Leuven, Belgium; Blake Hodges, Seifallah Ibrahim, Sabine O'Neal, Imec USA; Zsolt Tökei, Imec Belgium; Anna Herr, Quentin Herr, Imec USA**

The NbTiN films presented here are CMOS-compatible and were developed for metallization purposes in superconducting digital circuits [1-5]. Those circuits use NbTiN for Josephson junctions and capacitors electrodes, as well as for wiring. Superconducting digital circuits initially relied on Nb in the early days. NbTiN is a better candidate/replacement due to its higher thermal budget and better chemical stability [1-5]. In this study, the properties of superconducting NbTiN thin films deposited using two different sputtering methods have been compared. One method used multiple targets (MT) co-sputtering (Nb and Ti targets), while the other used a NbTi single target (ST). Benchmarking metrics used for comparison include: superconducting, electrical, as well as morphological properties. All films show a high T<sub>c</sub>, ranging from 13.3 K to 15.1 K. Compared to MT, ST NbTiN films showed consistently lower resistivity and better sheet

resistance (Rs) wafer-level uniformity (49 points wafer-map). For instance, 50 nm MT film had a Rs relative standard deviation (Stddev%) of 15.5%, while for the ST NbTiN films, Rs Stddev% showed a 2-fold improvement at 7.8%. Upon annealing of the ST NbTiN films at 650°C, the Rs uniformity further improved, reflected by a lower Stddev% at 4.5%. AFM data show similar results for MT and ST films, ~1.07 nm and 1.09 in the center and 0.73 nm and 0.71 nm at the edge of the wafers, respectively. Furthermore, XRD theta-2theta scans have been performed showing the 200 and 111 peaks for NbTiN orientations. Results show that the MT and ST films have different/signature 200/111 peak intensity ratios for the as deposited films. ST NbTiN films have a lower 200/111 peak ratio. However, after annealing at 650°C, the ST films 200/111 peak ratio increases, and surpasses that of the MT NbTiN films. This change suggests a change in the ST film disorder and grain size after annealing. The impact of the ST NbTiN film thickness on properties has also been studied. The T<sub>c</sub> shows an increase as a function of thickness, from 9.6 K for 7 nm, to 14.3 K for 50 nm, up to 14.9 K for 200 nm films. Certainly, the ability to tune the superconducting properties of NbTiN, makes them appealing from a stack engineering perspective. Both MT and ST NbTiN properties can be tailored using deposition conditions such as: power, partial pressure and post deposition annealing [3]. However, MT NbTiN films 300 mm wafer-level Rs non-uniformity represents a limiting factor for scaling superconducting devices. Annealed NbTiN ST films on the other hand, show a 3.4-fold Rs wafer uniformity improvement while maintaining properties tunability.

9:00am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-5 Controlling the Properties of Epitaxially Grown Topological Semimetals, Kirstin Alberi, National Renewable Energy Laboratory**

INVITED

Three dimensional topological semimetals (TSMs) exhibit a wide range of interesting properties, including high carrier mobility, large magnetoresistance, anomalous transport behavior, broadband optical absorption and non-linear optical responses. Epitaxial thin film synthesis offers a practical platform for manipulating composition, defects and disorder in these materials, offering a window into approaches for manipulating their properties. In this talk, I will discuss insights into the relationships between structure and composition and the resulting properties revealed through careful control of growth conditions. Focused examples include the impact of point defects and impurities on electron transport in the Dirac TSM Cd<sub>3</sub>As<sub>2</sub> and the formation and behavior of domain boundaries in the Weyl TSM TaAs.

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9:30am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-7 Photon Down-Conversion of Yb-Doped CsPb(Cl<sub>1-x</sub>Br<sub>x</sub>)<sub>3</sub> to Low-bandgap Metal Halide Perovskites, Yutong Ren<sup>2</sup>, Princeton University; Igal Levine, The Hebrew University of Jerusalem, Israel; Dan Oron, David Cahen, Weizmann Institute of Science, Israel; Antoine Kahn, Princeton University**

Quantum cutting represents a transformative strategy to mitigate thermalization losses that typically occur when high-energy photons are absorbed by semiconductors.<sup>1,2</sup> Recent advances have extended this concept from rare-earth doped crystals to semiconductor-rare-earth hybrid systems, particularly those utilizing halide perovskite absorbers, thereby exploiting their exceptional optoelectronic properties.

In this study, we focus on Ytterbium (Yb) -doped CsPb(Cl<sub>1-x</sub>Br<sub>x</sub>)<sub>3</sub>, a metal halide perovskite that absorbs visible light and exhibits intense near-infrared (NIR) photoluminescence—a clear signature of efficient quantum cutting. Upon excitation with visible light, the doped perovskite converts the absorbed energy into two NIR photons, with the emission energy closely matching the optimized bandgap of a Sn-Pb based perovskite absorber. This spectral alignment is critical for enabling effective energy transfer between the quantum cutting layer and the absorber.

<sup>1</sup> JVST Highlighted Talk

<sup>2</sup> JVST Highlighted Talk

Our investigation focuses on elucidating the structural and electronic properties of the interfaces between Yb-doped  $\text{CsPb}(\text{Cl}_{1-x}\text{Br}_x)_3$  and Sn-Pb based perovskite films. By employing a suite of advanced spectroscopic techniques—including ultraviolet photoelectron spectroscopy, inverse photoemission spectroscopy, time-resolved photoluminescence (tr-PL), and time-resolved surface photovoltage (tr-SPV)—we systematically examine how the quantum cutting layer, the absorber layer, and their interfacial region collectively influence energy transfer efficiency. In particular, the complementary tr-PL and tr-SPV analyses unambiguously determine the dominant interfacial charge transfer and recombination processes, and thus gain control over the interfacial charge transfer. By integrating Yb-doped  $\text{CsPb}(\text{Cl}_{1-x}\text{Br}_x)_3$  with customized Sn-Pb perovskite absorbers, our approach shows promise for pushing the boundaries of conventional efficiency limits while also offering a cost-effective strategy for enhanced energy conversion.

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9:45am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-8 Molecular Beam Epitaxy Growth of  $\text{InAs}_{1-x}\text{Bi}_x$  on GaSb for Topological Insulating States**, *Merve Baksi, James Rushing, Xikae Xie, Avery Hanna, Larry Qui, Ekow Williams, Paul J. Simmonds*, Tufts University

Incorporation of bismuth (Bi) into III-V semiconductors has attracted significant interest not only for its ability to extend infrared optoelectronic applications across a wide spectral range but also for its potential to induce topologically protected surface states, which could form the foundation for certain quantum computing technologies [1].

Motivated by the small inverted band gap that can be induced in  $\text{InAs}/\text{GaSb}$  quantum wells (QWs) [2], we propose engineering the band structure and inducing the edge states through Bi incorporation into  $\text{InAs}$  layers. This enhancement is expected to improve robustness against thermal fluctuations, making the material viable for room temperature applications as opposed to the topological  $\text{HgTe}/\text{CdTe}$  QW system with a temperature dependent band gap [3].

Theoretical studies predict that  $\text{InAs}_{1-x}\text{Bi}_x$  quantum wells exhibit a topological insulating state when the Bi composition reaches  $x \approx 0.15$ , with an estimated inverted gap of approximately 30 meV [1]. Given these predictions,  $\text{InAsBi}$  emerges as a promising candidate for realizing two-dimensional topological insulators (2D TIs). However, achieving such high Bi incorporation remains challenging due to the significant miscibility gap and the limited solubility of Bi in III-V materials [4].

In this work, we investigate the molecular beam epitaxy (MBE) growth of  $\text{InAsBi}$  on GaSb substrates, focusing on optimizing Bi incorporation and structural quality. By leveraging MBE growth techniques, we aim to systematically control Bi incorporation and assess its impact on electronic and structural properties of  $\text{InAsBi}$  in reduced dimensions. Our findings will contribute to the advancement of III-V-based topological materials and their potential integration into future quantum devices.

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## Electronic Materials and Photonics

### Room 207 A W - Session EM2+AP+QS+TF-TuM

#### Evolution of Materials and Devices for Energy Harvesting and Conversion

**Moderators:** Seth King, University of Wisconsin - La Crosse, Parag Banerjee, University of Central Florida

11:00am **EM2+AP+QS+TF-TuM-13 Structural and Electronic Properties of  $\text{CdSe}_x\text{Te}_{1-x}$  /CdTe thin-film photovoltaic devices: Carrier Dynamics Analysis by Charge Carrier Collection Efficiency**, *Philip (Sanghyun) Lee*, University of Kentucky; *Kent Price*, Morehead State University

Polycrystalline Cadmium Telluride (CdTe) thin-film solar cells are among the most successful commercial thin-film solar technologies, achieving a record cell efficiency of nearly 23.1% and offering competitive module costs compared to silicon (Si) modules. More than 20 GW of CdTe modules have been installed worldwide. Laboratory-scale tests have even surpassed 23.1%, getting closer to the theoretical Shockley-Queisser limit of about 32%. Recent research has focused on integrating selenium (Se) into CdTe absorbers to create band grading without the use of CdS window layers. The compound  $\text{CdSe}_x\text{Te}_{1-x}$  has emerged as a key candidate for enhancing the short-circuit current ( $J_{sc}$ ) by lowering the bandgap below 1.45 eV, which could help push short-circuit-current ( $J_{sc}$ ) closer to its theoretical limits.

In this study, we fabricated  $\text{CdSe}_x\text{Te}_{1-x}/\text{CdTe}$  devices with vapor transport technology (VTD) and characterized the structural chemistry and electronic properties of  $\text{CdSe}_x\text{Te}_{1-x}/\text{CdTe}$  devices from the carrier collection dynamics perspective. The device structure is  $\text{CdSeTe}/\text{CdTe}$  absorbers on TEC-10 glass coated with fluorine-doped tin oxide ( $\text{SnO}_2:\text{F}$ ), and finished with Gold back metal contact to minimize the impact of unwanted back contact Schottky barrier on carrier dynamics. The devices were treated under  $\text{Cl}_2$  ambient at 480 C for grain recrystallization and grain boundary passivation. Selenium (Se) diffuses deeper into the CdTe film to form  $\text{CdSeTe}$ . The device was then assessed using cross-section using Scanning Transmission Electron Microscopy (STEM) coupled with Energy dispersive X-ray analysis (STEM-EDX) in addition to evaluating device performance and characteristics. The carrier collection is measured by quantum carrier collection efficiency. The results indicate that Se uniformly diffused into CdTe grains, forming  $\text{CdSeTe}$ , which effectively lowers the bandgap energy to 1.41 eV, which is 40 mV lower than our initial calculation (1.45 eV), which increased photocurrent to 28.66 mA/cm<sup>2</sup>. The Se concentration is approximately 5-7 %, incorporated into the front interface of  $\text{CdSe}_x\text{Te}_{1-x}/\text{CdTe}$  films. From the carrier dynamics analysis, the total loss of charge carrier collection is 19.6%, as compared to ideal charge carrier collection at the front heterojunction of  $\text{CdSe}_x\text{Te}_{1-x}/\text{CdTe}$ . This indicates that there is room to further improve charge carrier collection to achieve higher photocurrent and, thus, efficiency. The UV and violet light charge collection is 5.46 mA/cm<sup>2</sup>, whereas the red light charge collection is 4.37 mA/cm<sup>2</sup>. The most charge collection occurs at in-between wavelengths as 18.71 mA/cm<sup>2</sup>.

11:15am **EM2+AP+QS+TF-TuM-14 Analysis of  $\text{KNbO}_3$  Crystal Structure Fabricated on  $\text{LiNbO}_3$  and  $\text{LiTaO}_3$  Substrate for Piezoelectric Sensors and Devices Applications**, *LAY THITHI, Asuki Hagiwara, Ryotsuke Arai, Josai University, Japan*

Recently, small scales energy harvester with clean energy sources are in demand for various portable sensors and electronics devices [1]. Piezoelectric materials such as  $\text{KNbO}_3$  are in focus for new type of sensors and electronic materials due to its high piezoelectric properties, high curie temperature around 450°C as well as lead free for environmental hazard compared to lead zirconate titanate PZT [2-3]. On the other hand, piezoelectric crystal such as lithium niobate ( $\text{LiNbO}_3$ ) and lithium tantalate ( $\text{LiTaO}_3$ ) also have been widely used in electronic and communication devices because it has high electro-optical properties as well as high curie temperature which is considered as the most important parameter for device performance [4]. In this study, well-ordered  $\text{KNbO}_3$  film were synthesis on  $\text{LiNbO}_3, \text{LiTaO}_3$  single crystals substrate by hydrothermal method aiming for possibility of electro-optical switching devices, energy conversion and other sensing devices.

$\text{KNbO}_3$  (100) and (111) structure epitaxially grown on  $\text{LiNbO}_3$  and  $\text{LiTaO}_3$  single crystal substrate with various reaction time and conditions. Crystal structure and film thickness were analyzed by SEM and XRD. Grains size ranging from 1-7µm and polycrystalline crystal film with thickness varies 3-10µm were obtained by single reaction. Two different substrates showed different surface morphology and crystal structure to understand lattice

matching  $\text{KNbO}_3$  film synthesis on  $\text{LiNbO}_3$  and  $\text{LiTaO}_3$  which is important for piezo electric properties [5].

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**11:30am EM2+AP+QS+TF-TuM-15 Modelling the Surface Electronic Properties of Catalytic Condenser for Programmable Reactions, Lars Grabow, Shengguang Wang, University of Houston; Kaida Liu, Ulrick Gaillard, University of Minnesota; Rohit Punyapu, Rachel Getman, Ohio State University; Matthew Neurock, University of Minnesota** **INVITED**

The evolution of catalyst design has progressed from structural control and optimization to dynamic electronic control of active sites for surface chemistry. This advancement enables precise tuning of active sites via potential, light, or strain applied to material surfaces. Catalytic condensers are novel devices that stabilize charge from an applied potential across a high- $\kappa$  dielectric film in a thin top layer of carbon with active sites on metal nanoclusters. This talk examines several computational methods to calculate charge condensation on catalytic condensers and the influence on the adsorption of atomic and molecular species.

The tested methods include direct quantum chemical cluster calculations, charged periodic calculations with homogeneous background counter charge, implicit solvation methods, localized countercharge within the vacuum region, and explicit charge transfer atoms within the vacuum region. Density functional theory (DFT) calculations were employed to evaluate these methods, providing insights into the influence of condensed charge on adsorption and assessing the accuracy and computational requirements of each approach.

The study systematically varied the charge on metal surface atoms from -1 to +1 per atom, calculating binding energies for atomic adsorbates such as H, O, N, and C, as well as the molecular adsorbate CO on ideal single crystal 3d, 4d, and 5d transition metal surfaces, namely Cu(111), Ru(0001), and Pt(111). The applicability of each method was explored by examining the range of systems that can be calculated, computational demands, accuracy of results, and potential pitfalls. Cluster calculations, periodic methods, and implicit solvation models were compared, revealing that charged periodic calculations with homogeneous background counter charge and large vacuum region provided the most practical and computationally efficient results. The study also highlights the role of electric fields versus charge, depicting the extent of polarization of adsorbates from charge density difference plots.

Overall, the choice of method remains a tradeoff between accuracy and computational expense. The findings offer general conclusions about catalytic condensers and contribute to the understanding of electronic control in catalytic surfaces, paving the way for future advancements in programmable catalyst design.

## Quantum Science and Technology Mini-Symposium

### Room 208 W - Session QS1-TuM

#### Quantum Simulations and Quantum-Inspired Technologies

**Moderator: Andre Schleife**, University of Illinois at Urbana-Champaign

**8:00am QS1-TuM-1 Investigating Processing Spaces of Epitaxially Grown Nitride Materials with Quantum and Conventional Supervised Learning, Andrew Messecar<sup>1</sup>**, Western Michigan University; **Kevin Vallejo**, Idaho National Laboratory; **Steven Durbin**, University of Hawai'i at Mānoa; **Brelon May**, Idaho National Laboratory; **Robert Makin**, Western Michigan University

The experimental design of material synthesis occurs within highly complex processing spaces defined by multiple design parameters. Traditional identification of optimal values for each design term often involves an iterative, costly, Edisonian trial-and-error strategy for experiment design. Therefore, there is great interest in leveraging machine learning-based approaches to enhance and expedite the strategic design of materials and their synthesis pathways. Here, information describing plasma-assisted molecular beam epitaxy (PAMBE) growth trials of transition metal and group-III nitrides have been organized into distinct, composition-specific data sets. For each synthesis record, the complete recipe of experiment design parameters (substrate temperature, element source conditions, growth duration, etc.) are associated with binary numerical labels representing sample crystallinity and surface morphology as determined via *in-situ* reflection high-energy electron diffraction (RHEED) patterns. A Bragg-Williams measure of lattice ordering ( $S^2$ ) is also investigated as an additional, continuous figure of merit pertaining to atomic-scale disorder. Quantum and classical machine learning algorithms – including linear models, neural systems, tree-based algorithms, and quantum support vector machines – are fit to the data to investigate which growth parameters have the most statistically significant influence over each material property of interest. When predicting the occurrence of monocrystalline PAMBE-grown GaN sample surfaces, supervised learning techniques incorporating quantum computation display notable generalization advantage when compared to classical machine learning approaches. The class-conditional probabilities of obtaining single crystalline, atomically-flat thin film crystals – as well as the degree of lattice ordering measured by  $S^2$  – are forecasted across broad ranges of possible PAMBE operating parameter combinations. These predictions are compared to experimental best practices as well as the results described in published literature detailing the PAMBE synthesis of these materials. The improved generalization performance displayed by the quantum-aware models when predicting GaN crystallinity implies a potential advantage gained via quantum computational studies of synthesis-property relationships in other material systems.

<sup>\*</sup>This work was supported in part by the United States Department of Energy (award number DE-SC0025835) as well as the National Science Foundation (grant number DMR-2003581).

**8:15am QS1-TuM-2 Quantum Simulation of Spin-Current Autocorrelation Function, Yi-Ting Lee**, University of Illinois at Urbana Champaign; **Bibek Pokharel**, IBM, T.J. Watson Research Center; **Arnab Banerjee**, Purdue University; **Andre Schleife**, University of Illinois at Urbana-Champaign; **Jeffrey Cohn**, IBM Almaden Research Center

Understanding spin dynamics has long intrigued physicists, as it plays a vital role in revealing the characteristics of quantum magnets, with potential applications in spintronic devices and spin qubits. Evaluating the dynamical properties of large spin systems is often challenging for classical computers due to the exponential growth in memory requirements. Since Hamiltonian dynamics can be efficiently simulated using quantum circuits, the evaluation of time-dependent properties has generated significant interest within the quantum computing community.

While time-dependent magnetization and the one-time dynamical structure factor have been simulated on quantum computers before, there has been no simulation of the spin-current autocorrelation function (ACF). The one-time spin-current ACF can be used to identify the diffusion behavior of spin systems and is directly related to their coherence properties and device performance. In this research, we first consider the spin-1/2 XXZ Heisenberg model as it serves as the framework for studying magnetic interaction.

Here, we introduce a simple yet efficient direct measurement scheme for evaluating the one-time spin-current ACF. Unlike the standard Hadamard

<sup>1</sup> AVS Dorothy M. and Earl S. Hoffman Scholarship Recipient



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test, our method eliminates the need for control gates with ancilla qubits and reduces the number of required circuits by a factor of  $N$ , where  $N$  is the number of qubits. We demonstrate the circuit design and measurement protocol and validate it through a quantum experiment on the *ibm\_marrakesh* hardware. In the 20-qubit experiment with the Néel state, we achieve excellent agreement with the numerical results for both the real and imaginary parts, highlighting the effectiveness of our method. Moreover, we present a design for measuring the two-time spin-current ACF and demonstrate good agreement between statevector-simulated results and numerical results, further showcasing the utility of our approach. Furthermore, our method can be potentially extended to measure any ACF, benefiting the study of spin dynamics.

This work is supported by Taiwan UIUC scholarship, and we acknowledge support by the IBM Illinois Discovery Accelerator Institute and the IBM Extenship Program. This work made use of the Illinois Campus Cluster, a computing resource that is operated by the Illinois Campus Cluster Program in conjunction with the National Center for Supercomputing Applications and which is supported by funds from UIUC. The research at IBM and Purdue is supported by National Quantum Initiative Science Research Centers, Quantum Science Center, managed by ORNL for the US-DOE.

**8:30am QS1-TuM-3 Quantum Information Processing Stack: From Bottom to Top and Back**, *Sophia Economou, Karunya Shiral, Virginia Tech* **INVITED**  
Quantum processors have become quite large and sophisticated machines over the last several years, with many tech companies racing to develop the first quantum computer of practical utility. While the progress has been impressive, quantum processors still face significant hurdles such as short coherence times and high error rates. They are not yet able to compete with classical information processing technologies in solving problems of practical interest. I will discuss my group's contributions across the quantum information processing stack, from the control of quantum hardware to quantum algorithm development and back.

**9:15am QS1-TuM-6 Quantum-Enhanced Communication Network Routing in Cyber-Physical Power Systems**, *Shuyang Ma, Yan Li, Penn State University*

Communication networks in cyber-physical power systems play a vital role in ensuring reliable information exchange, enabling real-time monitoring, control, and coordination of distributed energy resources. However, ensuring real-time responsiveness while meeting strict Quality of Service (QoS) constraints, such as low latency and high reliability, introduces significant challenges. A central problem is the constrained shortest path (CSP), which seeks to minimize communication costs across the grid while adhering to a maximum delay threshold. This NP-hard problem becomes computationally infeasible for large-scale networks using conventional approaches. To tackle this, we propose a novel method that transforms the CSP problem into a Quadratic Unconstrained Binary Optimization (QUBO) model, subsequently mapped to an Ising Hamiltonian. This reformulation enables the use of the Quantum Approximate Optimization Algorithm (QAOA), a hybrid quantum-classical technique that exploits quantum parallelism to efficiently approximate optimal routing solutions. Our approach offers reduced computational complexity and improved scalability compared to traditional methods. Through numerical simulations, we demonstrate that this QAOA based strategy successfully identifies cost-effective paths that satisfy QoS requirements, underscoring its potential to revolutionize network optimization in power grids as quantum computing advances.

**9:30am QS1-TuM-7 Floquet-ADAPT-VQE: A Quantum Algorithm to Simulate Non-Equilibrium Physics in Periodically Driven Systems**, *Abhishek Kumar, Karunya Shiral, Nicholas J. Mayhall, Sophia E. Economou, Edwin Barnes, Virginia Tech*

Non-equilibrium many-body quantum systems exhibit many fascinating phenomena absent in equilibrium systems, but simulating them on classical computers is challenging. We propose a hybrid quantum-classical algorithm, Floquet-ADAPT-VQE, to simulate the non-equilibrium physics of periodically driven quantum systems. We utilize the Floquet-Hilbert space, a composition of auxiliary and physical spaces, to transform the Hamiltonian into a time-independent form. We define a cost function based on the square of the shifted extended Floquet Hamiltonian and show how to prepare Floquet eigenstates using Floquet-ADAPT-VQE. We also obtain a suitable auxiliary initial state whose squared Floquet energy is independent of the number of auxiliary qubits as well as the driving frequency, which leads to better convergence with fewer ADAPT iterations. Additionally, we provide a framework to calculate the time-dependent expectation value of observables in the Floquet state with fixed-depth quantum circuit. We

demonstrate our algorithm by performing numerical simulations on a periodically driven XYZ model with a magnetic field. We also explore potential applications of our algorithm for studying various non-equilibrium phenomena in periodically driven systems.

## Quantum Science and Technology Mini-Symposium Room 208 W - Session QS2-TuM

### Quantum Foundries, Educational Initiatives, Sensing and Metrology

**Moderators:** Ekta Bhatia, NY CREATES, Haozhi Wang, University of Maryland College Park

**11:00am QS2-TuM-13 NIST on a Chip, Quantum-Based Sensors for Metrology in the Quantum Era**, *Jay Hendricks, National Institute of Standards and Technology (NIST)* **INVITED**

The re-definition of the SI units enables new ways to realize fundamental units. Quantum-based metrology systems, however exciting, do raise new challenges and several important questions: Can these new realizations enable the size and scale of the realization to be miniaturized to the point where it can be imbedded into everyday products? What will be the role of metrology institutes in the new ecosystem of metrology and measurement? This talk will begin to explore these important philosophical questions. The technical core of the talk will be a deeper dive into research on measurement methods for pressure, the Fixed Length Optical Cavity (FLOC) and for vacuum the Cold Atom Vacuum Standard (CAVS). What is exciting about many of these new measurement approaches is that they are both primary (relying on fundamental physics), are quantum-based and use photons for the measurement readout which is key for taking advantage of the fast-growing field of photonics.

**11:30am QS2-TuM-15 RF Imaging of Sub-Surface Defects in Si(100) with an STM Tip-Induced Quantum Dot**, *Jonathan Marbey, Michael Dreyer, Matthew Brooks, University of Maryland; Omadillo Abdurazakov, Yun-Pil Shim, University of Texas at El Paso; Robert Butera, Laboratory for Physical Sciences (LPS)*

We present radio frequency (RF) reflectometry measurements that have been combined into a millikelvin scanning tunneling microscope (mK-STM). This technique is realized through a relatively straight forward integration of an LC tank circuit into the STM tip-plate. For semi-conductor samples, application of a voltage bias gives rise to tip-induced band bending which leads to the formation of an induced quantum dot that can be scanned across the sample surface. This measurement geometry provides a unique detection method, as variations in the energy of a state confined to the tip-induced quantum dot due to the local environment leads small changes in quantum capacitance. These capacitance variations can be effectively sensed via RF reflectometry of the tunnel junction provided the tank circuit has a sufficient quality factor  $Q$ . In particular, we find strong phase contrast in the presence of resonant tunnel coupling between the induced dot and sub-surface defect states. As a demonstration of this capability, we present experimental results on highly phosphorus doped ( $10^{19}\text{cm}^{-3}$ ) Si(100). 1-D voltage dependent spectroscopy measurements in the vicinity of defects reveal ring-like structures in the reflected phase that can be effectively modeled by an asymmetric double-dot detuning picture. This technique ultimately aims to emulate read-out geometries relevant to modern quantum dot devices.

**11:45am QS2-TuM-16 Pushing the Boundaries of Coherence in Superconducting Quantum Systems at the SQMS Center for Computing, Sensing, and Metrology**, *Tanay Roy, Fermi Lab* **INVITED**

This talk will highlight recent advances at the SQMS Center in understanding and mitigating decoherence in superconducting quantum systems, focusing on both transmon qubits and 3D superconducting cavities. I will present results from systematic studies of materials and devices, aimed at identifying key sources of loss: including two-level systems (TLS), quasiparticles, and other noise mechanisms. These studies span microwave loss characterization in materials such as niobium, tantalum, aluminum, and their native oxides, as well as substrate losses in silicon and sapphire. Using both qubits and cavities, we disentangle subsystem contributions to loss and develop a hierarchy of mitigation strategies. Through these efforts, we have achieved transmon coherence times exceeding one millisecond. I will also present investigations into quasiparticle dynamics, including bursts observed in qubits located above ground and in the Gran Sasso underground laboratory. Additional studies explore temperature dependence to distinguish between TLS and

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quasiparticle losses, and reveal that applying a magnetic field can reduce temporal  $T_1$  fluctuations in transmons.

Building on these results, we demonstrate a record-coherence two-cell cavity-qudit system with coherence times exceeding 20 milliseconds. By leveraging sideband interactions and error-resilient protocols—including measurement-based correction and post-selection, we achieve high-fidelity quantum state control. This includes preparation of Fock states up to  $N = 20$  with fidelities over 95%, and two-mode entanglement with coherence-limited fidelities reaching 99.9% after post-selection. These achievements position the SQMS platform as a powerful foundation for scalable quantum information processing and high-dimensional qudit encodings. Finally, I will discuss how these ultra-coherent systems are being deployed in emerging quantum sensing applications, including dark matter searches and gravitational wave detection.

## Quantum Science and Technology Mini-Symposium Room 208 W - Session QS1-TuA

### Interdisciplinary Quantum Applications

**Moderators:** Yi-Ting Lee, University of Illinois at Urbana Champaign, Kasra Sardashti, University of Maryland College Park

**2:15pm QS1-TuA-1 A Study of Superconducting Behavior in Ruthenium Thin Films, Bernardo Langa Jr.,** University of Maryland; **Brooke Henry,** Clemson University; **Ivan Lainez,** University of Maryland; **Richard Haight,** IBM; **Kasra Sardashti,** University of Maryland

Ruthenium (Ru) is a promising candidate for next-generation electronic interconnects due to its low resistivity, small mean free path, and superior electromigration reliability at nanometer scales. In addition, Ru exhibits resistance to oxidation, low diffusivity, and most importantly, superconductivity below 1 K. These qualities make Ru an attractive material for superconducting qubits where its stability may help mitigate two-level system defects. Here, we investigate the superconducting behavior of Ru thin films (11.9–108.5 nm thick), observing transition temperatures from 657.9 mK to 557 mK. A weak thickness dependence appears in the thinnest films, followed by a conventional inverse thickness dependence in thicker films. Magnetotransport studies reveal type-II superconductivity in the dirty limit ( $\xi > l$ ), with coherence lengths ranging from 13.5 nm to 27 nm. Finally, oxidation resistance studies confirm minimal RuOx growth after seven weeks of air exposure. Our findings provide key insights for integrating Ru into superconducting electronic devices and explore its potential in advancing scalable, high-coherence quantum devices.

**2:30pm QS1-TuA-2 Realizing Epitaxial Trilayer Josephson Junctions Grown with Molecular Beam Epitaxy, Colin Myers,** University of Maryland, College Park; **Kasra Sardashti,** Laboratory for Physical Sciences; **Christopher Richardson,** Laboratory for Physical Sciences, College Park

The Al/AlOx/Al Josephson Junction (JJ) remains the primary choice for superconducting qubit design. Reducing the potential loss mechanisms and two-level systems (TLS) in these junctions is a major priority for quantum computation and design. Hence, many alternatives to the traditional JJ are being explored, with NbTiN posing as a possible substitute for aluminum. Alloyed NbTiN possesses a  $T_c$  near 17 K, allowing for far higher operating temperatures compared to aluminum. Utilizing plasma-assisted molecular beam epitaxy (PAMBE), we grow epitaxial trilayer stacks of NbTiN/AlN/NbTiN, where AlN serves as the insulating barrier layer of the JJ. This allows for an oxygen-free system, in addition to employing the precise thickness and compositional control associated with traditional MBE growth. Assembling a JJ from this trilayer architecture now presents unique patterning and lithography challenges. We present a novel approach to JJ design and fabrication, as well as epitaxial NbTiN as an emergent material for quantum information science.

**2:45pm QS1-TuA-3 Enabling Quantum Information Science with DNA-Templated Quantum Materials, Xin Luo<sup>1</sup>, Jeffrey Gorman, Mark Bathe,** Massachusetts Institute of Technology

Quantum information science is limited by the lack of materials that enable precise, rational control over quantum photonic, excitonic, and spin states and other properties of the quantum materials. While DNA nanotechnology offers in principle such control via spatial templating of chromophores, quantum dots, and molecular spin centers with nanometer-scale precision, this capability requires interfacing with silicon-based 2D devices to enable quantum information science with translational impact on devices. Toward this end, we previously demonstrated that programmable DNA templates can position quantum materials such as colloidal quantum dots and rods with nanometer-scale precision for integration with photonic devices through top-down electron beam lithography [1]. Here, we apply this approach to fabricate photonic cavities to control single-photon emissive properties and photonic waveguides for photonic quantum circuits. We additionally demonstrate pathways towards controlling molecular spins and excitons with DNA templates for quantum information science and technology. This scalable approach to templating quantum materials opens new applications to quantum sensing, networking, and simulation, with potential impact on secure communications, medical diagnostics, computing, and beyond.

[1] Luo, X. *et al.* DNA origami directed nanometer-scale integration of colloidal quantum emitters with silicon photonics. *bioRxiv*, doi: 10.1101/2025.01.23.634416 (2025).

**3:00pm QS1-TuA-4 Enhanced Readout Contrast of V2 Ensembles in 4H-SiC Through Resonant Optical Excitation, Infiter Tathfif,** University of Maryland College Park; **Charity Burgess, Brenda VanMil,** Army Research Laboratory; **Samuel G. Carter,** Laboratory for Physical Sciences

Favorable optical and spin properties of the V2 silicon vacancy defect in 4H-SiC have made it a promising candidate for quantum technologies. For quantum sensing with defect spins, the contrast in optically-detected magnetic resonance (ODMR) is an important metric, which tends to be rather low (<1%) for V2 ensembles using off-resonant laser excitation. To improve contrast, we resonantly excite the V2 ensembles at low temperatures and compare our findings with off-resonant excitation. Our measurements show a ~90 times improvement for ODMR contrast over the off-resonant case for fairly low resonant excitation. We hypothesize that for a particular wavelength, the resonant laser excites a subset of defects within the ensemble and drives only one of the spin-selective optical transitions for each defect. This leads to a strong spin polarization, contributing to the high readout contrast. To test our hypothesis and further characterize the behavior, we examine the dependence of the contrast on the laser linewidth and the sample temperature. Modulating the resonant laser linewidth up to 1 GHz, corresponding to the splitting of the two optical transitions, results in the contrast decreasing by 50%. As the temperature is increased to 60 K, the contrast decreases and reaches the off-resonant value, presumably due to linewidth broadening. Although the PL signal is 50 times weaker than the off-resonant excitation due to the participation of the defect sub-ensemble, the sensing figure of merit (FoM) is 10 times higher, making the resonant approach still the best choice for sensing at low temperatures. Due to the high readout contrast and reduced laser power requirements, we plan to utilize this resonant technique for wide-field magnetic imaging of quantum materials and devices at low temperatures.

**3:15pm QS1-TuA-5 Enhancement of Superconductivity in Cryogenically Grown Ultra Thin Al Films, Teun van Schijndel, Yu Wu, Wilson Yáñez-Parreño, Tawshia Chowdhury, Christopher Palmstrom,** University of California at Santa Barbara

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

## Quantum Science and Technology Mini-Symposium Room 208 W - Session QS2-TuA

### Scalable Fabrication for Quantum Technology

**Moderators:** Ekta Bhatia, NY CREATES, Bernardo Langa, Jr., University of Maryland

**4:00pm QS2-TuA-8 Sandia's Approach to Scalable Single Defect Center Creation using Focused Ion Beam Implantation, Edward Bielejac,** Sandia National Laboratories

INVITED

We will present an overview of Sandia's Ion Beam Laboratory (IBL) and its ongoing efforts to develop focused ion implantation capability using a range of accelerators to create scalable defect centers in wide bandgap materials. This presentation will cover three main topics:

<sup>1</sup> JVST Highlighted Talk

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(1) Novel liquid metal alloy ion source development (LMAIS) where we will concentrate on the development of LMAIS for our two mass filtered Focused Ion Beam (FIB) systems, the A&D nanomplanner (A&D FIB100NI) and the Raith Velion, both of which combine high spatial resolution with CAD based patterning to enable the formation of arbitrary patterned implantation in a wide range of substrates.

(2) In-situ counting and in-situ photoluminescence (PL) to enable single defect center creation in wide bandgap materials such as diamond and silicon carbide. Using in-situ counting we demonstrate a seven-fold improvement on the expected ion implantation error over timed implantation. Using in-situ PL we enable real-time error correction on the formation of low yield optically active defect centers. The combination of counting and PL is a promising pathway towards deterministic formation of these defect centers.

(3) The development of ultra-low energy ( $<1$  keV) focused ion implantation capability based on a biased sample holder configuration. This enables ultra-low energy implantation while maintaining an expected implantation resolution of between 100-300 nm.

It is the combination of these three topics that fundamentally enables the IBL approach to scalable single defect creation using FIB implantation.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

**4:30pm QS2-TuA-10 Scalable Single-Erbium Ion Qubits in Silicon Carbide for Integrated Photonics in the Telecom Band, Spyros Galis, Alexander Kaloyeros, University at Albany-SUNY**

Advancing quantum photonics and communications requires scalable optical quantum devices compatible with chip-scale device integration and higher temperature operation ( $\geq 77$  K) for integration into photonic integrated circuits (PICs). Highly integrable silicon carbide (SiC) has emerged as a promising PIC platform, offering ideal material and optical properties for classical and quantum photonics. In parallel, scalable material platforms doped with erbium ( $\text{Er}^{3+}$ ), which has an optical transition in the telecom range at  $\sim 1532$  nm, can enable a plethora of exciting photonic and quantum technologies operating in the telecom C-band. Toward this, telecom single-photon emitters (SPEs) and qubits based on single ions in semiconductors are essential for quantum PICs (qPICs), yet scaling them beyond the lab remains challenging due to material constraints, stringent fabrication and temperature requirements, and random emitter placement, complicating PIC integration.

Our approach utilizes a novel, scalable nanofabrication scheme to address these challenges, enabling the creation of SiC nanowires (NWs) and hollow nanopillars (HNPs). This approach facilitates the following key-enabling innovations: 1) the precise ( $<5$  nm) placement of  $\text{Er}^{3+}$  ions in these nanostructures via advanced nanofabrication and implantation engineering and 2) an enhanced effective excitation cross-section ( $\sim 6 \times 10^{-18}$  cm<sup>2</sup>). By leveraging these innovations, we have successfully isolated and characterized single and few-erbium ions in SiC NWs and HNPs at temperatures of  $\geq 77$  K—otherwise unattainable in bulk materials. Furthermore, through nanofabrication engineering and the minimization of implantation-induced defects, we have demonstrated single-photon  $\text{Er}^{3+}$  emission with a narrow optical linewidth of 90 MHz and single- $\text{Er}^{3+}$ -ion qubit control, performed by Rabi oscillations in the optical domain and at temperatures of  $\geq 77$  K, in HNP SiC structures. Pertinent results will be presented, which, to our knowledge, represent the first experimental demonstrations of solid-state SPEs and single-ion qubits based on isolated  $\text{Er}^{3+}$ , highlighting our platform's viability for higher-temperature operation. We also concisely discuss opportunities for realizing Er-based SiC quantum integrated devices with improved performance and functionality, aiming to achieve practical qPIC devices for quantum and nanophotonic applications at telecom wavelengths.

**4:45pm QS2-TuA-11 Scalable, Precise, and Reliable Positioning of Colour Centres for Quantum Computing and Simulation, Mark Mills, Gianfranco Aresta, Kristian Stockbridge, Kate McHardy, Paul Blenkinsopp, Ionoptika Ltd., UK**

Quantum computing has the potential to revolutionize many aspects of modern technology and colour centres in diamond are a well suited system to be used as quantum simulators, quantum sensors and quantum networking interfaces. Nitrogen Vacancy (NV) centres are the most extensively studied due to their ground-state spin's long coherence times at

room temperature. Next to NV centres, also group-IV colour centres in diamond offer a promising platform for quantum networks and started gathering interest as an alternatives, with the Tin Vacancy (SnV) centres standing out among group-IV defects due to their optimal spin-orbit coupling.

The technological challenges related to the fabrication of quantum devices based on these systems are related to the reliable and precise positioning of N and Sn atoms into the diamond matrix and the subsequent post implantation process such as thermal annealing and the scalability of the whole process.

In 2024 Ionoptika Ltd started a joint development project, partially funded by Innovate UK, in partnership with Surrey University, Fraunhofer Institute for Applied Solid State Physics IAF and XeedQ GmbH, bringing together a Focused Ion Beam (FIB) System company, experienced FIB users and materials research Institutes with a quantum computing company. The aim of this project is to define a process for Scalable, Precise, And Reliable positioning of colour centres (NV and SnV) for Quantum computing and simulation.

We will be reporting on the engineering of a novel ion-beam column based on the well-established Ionoptika's Q-One platform for ion implantation. This single novel column will allow for use of both Liquid Metal Alloy Ion Source and Plasma Source. It will be equipped with an automated source adjustment system and ion beam autotuning. Parallel studies are being carried out with existing Q-One systems at Surrey University in collaboration with the other partners, Fraunhofer IAF and XeedQ, within this project, and we will report on these. We will also report on colour centres formation results obtained by other research institutes by using the Q-One ion implanter.

**5:00pm QS2-TuA-12 Integration of Atomic Precision Solid State Quantum Hardware with energy efficient circuit, architecture and algorithm co-design for Energy Efficiency Scaling, Tina Kaarsberg, Department of Energy; Sadasivan Shankar, SLAC National Accelerator Laboratory; Scott Lockledge, Tiptek**

It is auspicious that this abstract is being submitted on April 14—World Quantum Day—a date that includes the first three digits of Planck's constant, which is a fundamental constant in quantum physics. The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) multi-organization initiative to reduce computational energy use with energy efficiency scaling for two decades (EES2) will likely rely in part on advances in quantum computing—including quantum hardware to reach its ultimate 1000X energy efficiency goal. Under this initiative, DOE/AMMTO has funded analysis identifying new breakthrough approaches to energy efficient computing. For example, in Summer 2023, a SLAC analysis showed that using quantum algorithms for quantum mechanical calculations could use as little as one thousandth the energy of the same calculation on a classical computer. AMMTO also supports quantum hardware, for example in 2024, it announced two SBIR grants for qubit manufacturing development of 3D atomically precise (AP) qubits made using hydrogen depassivation lithography. Such AP qubits have inherently lower error rates than more macro-sized qubits. This paper will highlight co-design integration of such AP solid-state quantum hardware with quantum software. The co-design will include innovations in circuit, architecture and algorithm for a wide range quantum calculations that could enable DOE to reach its 1000X energy efficiency goal.

**5:15pm QS2-TuA-13 Measurement of Dielectric Loss in Piezoelectric Materials for Hybrid Quantum Systems, Ivan Lainez, University of Maryland College Park; Richard Mattish, Clemson University; Bernardo Langa, Jr., University of Maryland College Park; Maggie Marte, Deepak Sapkota, Clemson University; Christopher Rouleau, Jong Keum, Oak Ridge National Laboratory; Ashish Alexander, Laboratory for Physical Sciences; Kasra Sardashti, University of Maryland College Park**

An approach has been emerging to create hybrid quantum devices by combining quantum devices realized in distinct physical systems and therefore combining their advantages. In particular, piezo-acoustic cavities are of particular interest as they are capable of direct coupling of systems operating in the microwave regime to systems operating at the acoustic regime via acoustic modes through piezoelectric modulation. However, creating a piezo-acoustic cavity requires on-chip integration of physically disparate piezoelectric and superconducting materials while maintaining a coherent behavior at microwave frequencies and millikelvin (mK) temperatures. The extent of dielectric loss in the piezoelectric elements within the cavities has not been well studied. Here, we study the dielectric loss in epitaxial heterostructures of barium titanate (BTO), Strontium

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titanate(STO), and Lanthanum nickel oxide (LNO)-on-silicon as promising platforms for piezo-acoustic cavities. We use a 6-resonator superconducting coplanar waveguide design as a pilot device to measure microwave losses at mK temperatures. By changing the thickness of various layers within the BTO/Si, STO/Si, and LNO/Si heterostructures, including the buffer layers (e.g., YSZ, CeO<sub>2</sub>), we determine the loss contributions for each oxide layer. Microwave transmission for each chip is measured at 30 mK-2 K with powers ranging from -60 to -120 dBm. The transmission spectra are then analyzed to extract the actual resonant frequency, quality factors (internal vs. external), and effective dielectric constant for each chip.

## 2D Materials

Room 208 W - Session 2D+EM+NS+QS+SS+TF-WeA

### 2D Materials: Synthesis and Processing

Moderator: Tiancong Zhu, Purdue University

2:15pm **2D+EM+NS+QS+SS+TF-WeA-1 Process Discovery for Quantum Materials, *Stephan Hofmann***, University of Cambridge, UK **INVITED**

Effective heterogeneous integration of low-dimensional nanomaterials in applications ranging from quantum electronics to biomedical devices requires a detailed understanding of different formation and interfacing reactions and the ability to synergize these processes. Process development largely still follows an Edisonian trial-and-error approach, blind and constrained by conventional reactors. This is not only wasteful and frustratingly slow, but hinders scientific breakthroughs in crystal growth and innovation in new deposition technology. This talk will focus on our cross-correlative, high-throughput operando approaches and combinatorial close-space sublimation (CSS) based process design to accelerate process discovery. We show operando spectroscopic imaging ellipsometry and scanning electron microscopy with machine-learning assisted analysis and parameter space exploration for salt-assisted WS<sub>2</sub> layer CVD and TMD oxidation phenomena, and how direct kinetic process data can open data driven approaches to advance the required understanding of underpinning mechanisms.[1] We show that CSS is a highly promising alternative to conventional powder-furnace chemical vapour deposition, offering superior efficiency, precise structural control, scalability, and adaptable process designs. As part of processability and stability assessment, we also explore oxidation kinetics of TMD materials, [2] aided by atomistic modelling using machine-learned force fields.[3]

[1] Yang et al., Chem. Mat. 37, 989 (2025)

[2] Sahota et al., ACS Appl. Nano Mat., asap (2025)

[3] Gsanyi et al., arXiv:2401.00096, 2023

2:45pm **2D+EM+NS+QS+SS+TF-WeA-3 Selective Area Epitaxy of van der Waals Materials, *Ryan Trice***<sup>1</sup>, *Stephanie Law*, Penn State University

Two-dimensional (2D) van der Waals (vdW) materials are interesting for a variety of applications, ranging from optoelectronics and photocatalysis to energy storage and topological devices. However, vdW materials synthesized using common techniques like chemical or physical vapor deposition often have a high density of growth-related defects, including grain boundaries, twin defects, pyramidal growth, and spiral defects. While pyramidal growth can be minimized through higher growth temperatures, grain boundaries, twin defects, and spiral defects are much harder to overcome. For many applications, especially in electronics and optics, these defects lead to non-radiative recombination, electron scattering, and other undesirable effects. Furthermore, the fabrication of 2D materials into quantum dots (QDs) through bottom-up methods faces problems with precise location placement and polydispersity in the QDs' diameters. This makes the QDs difficult to characterize and is not ideal for most quantum computing and optical setups. Top-down nanofabrication approaches fix this issue but often cause significant damage to the surfaces or edges of the materials. To address these issues, we used molecular beam epitaxy (MBE) combined with selective area epitaxy (SAE) to grow Bi<sub>2</sub>Se<sub>3</sub> thin films. SAE is a technique in which thin films nucleate and grow in defined areas on a wafer. This is done using a patterned mask where growth conditions are selected such that the film will only nucleate on the substrate.

In this talk, we will describe SAE growth of Bi<sub>2</sub>Se<sub>3</sub> on Al<sub>2</sub>O<sub>3</sub> (0001) and Si (111) substrates using an atomic layer deposition SiO<sub>2</sub> mask. Etching of the SiO<sub>2</sub> mask was done with a wet chemical etch, resulting in micron-scale holes of various shapes and sizes. The processed substrates were then loaded into an MBE chamber for the growth of the Bi<sub>2</sub>Se<sub>3</sub> film. First, we will discuss the effects of different substrate temperatures on the selective growth of the Bi<sub>2</sub>Se<sub>3</sub> thin films. Second, we will discuss the geometric influence of various shaped patterns on the crystal quality of the selectively grown films. Third, we will look at the effect and viability of nano-scale patterns for selective growth of vdW materials. Further studies will focus on using different materials for the substrate and mask. This approach could allow us to grow wafer-scale, defect-free 2D vdW QDs at specified areas on the wafer, thereby increasing the scalability and applicability of these materials to real-world challenges.

3:00pm **2D+EM+NS+QS+SS+TF-WeA-4 Precision Synthesis and Conversion of 2D Materials by Pulsed Laser Deposition with in Situ Diagnostics, *Daniel T. Yimam***<sup>2</sup>, *Sumner B. Harris*, Oak Ridge National Laboratory, USA; *Austin Houston*, University of Tennessee Knoxville; *Ivan Vlassiouk*, Oak Ridge National Laboratory, USA; *Alexander Poretzky*, Oak Ridge National Laboratory; *Gerd Duscher*, University of Tennessee Knoxville; *Kai Xiao*, Oak Ridge National Laboratory, USA; *David B. Geohegan*, University of Tennessee Knoxville

Over the past few decades, 2D monolayers and heterostructures have become central to nanoscience, offering promising applications in electronics, sensing, and future computing. In addition to their exciting functional properties, significant progress has been made in their bottom-up synthesis and subsequent processing. Techniques such as encapsulation, doping, and implantation in atomically thin 2D materials are crucial to transitioning them from fundamental research to scalable, real-world applications, while enabling the emergence of novel properties. However, the ultrathin nature that makes 2D materials attractive also poses substantial challenges for traditional plasma-based processing methods. To fully harness the potential, it is essential to develop reliable processing techniques that offer precise control and reproducibility.

Pulsed laser deposition (PLD) is a promising non-equilibrium method that allows precise control over the kinetic energy (KE) of ablated species. In this work, we investigate plasma plume interactions with 2D materials using *in situ* plasma diagnostics and optical characterization tools. We demonstrate that a deep understanding and control of plasma plume dynamics enables new approaches for 2D material engineering, including the formation of Janus monolayers, metal atom implantation, and encapsulation with minimal damage. Our approach allows for low temperature substitution and implantation of foreign atoms, such as chalcogens and metals, facilitating the selective synthesis of Janus monolayers and alloys. These findings highlight the potential of PLD to drive the practical advancements in 2D materials for microelectronics and quantum information science.

This work was supported by the U.S. DOE, Office of Science, Materials Sciences and Engineering Division and the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

**Keywords:** Pulsed laser deposition, chalcogenide substitution, 2D materials, implantation, in situ diagnostics.

3:15pm **2D+EM+NS+QS+SS+TF-WeA-5 AVS Peter Mark Memorial Award Talk: Exploiting Thin Film Phase Diagrams for Synthesizing 2D Transition Metal Dichalcogenides, *Nicholas R. Glavin***, Air Force Research Laboratory **INVITED**

Synthesis of 2D transition metal dichalcogenides for specific applications in electronics, optoelectronic, and advanced coatings remains a critical bottleneck for many industrial applications. In this talk, we will highlight leveraging thin film phase diagrams to rapidly explore the vast parameter space in synthesizing these novel materials. This technique uses laser processing to locally modify regions within the film and coupled with high throughput characterization, rapidly assesses material state and quality for next generation sensors, optical coatings, and low power electronics.

4:15pm **2D+EM+NS+QS+SS+TF-WeA-9 Designer van der Waals Materials for Quantum Optical Emission, *Shengxi Huang, Wenjing Wu***, Rice University **INVITED**

Designer van der Waals (vdW) materials offers enormous opportunities to tune material properties for various applications. Isolated, optically-active defects generated in vdW materials could lead to single photon emission. 2D vdW materials as host materials for single photon emission hold various advantages, such as high optical extraction efficiency from the atomically-thin layered materials, and readiness to integrate with on-chip photonic and electronic devices. However, single photon emission from 2D vdW materials typically suffers from low purity and lack of controllability, due to the sensitivity of these atomically-thin materials to external dielectric environments, surface defects and adsorbents, and strains and wrinkles introduced during material processing. This talk introduces our recent efforts to improve the single photon purity and controllability in vdW materials. We developed novel defect structures that can overcome several current issues, and explored their electronic structure and tunability in optical emission. Through a combination of approaches, including strain engineering, heterostacking, employing optical selection rules for excitation and detection, optimization of material synthesis and handling, we were able to achieve high purity (> 98%) for single photons emitted from 2D

<sup>1</sup> JVST Highlighted Talk

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<sup>2</sup> JVST Highlighted Talk

transition metal dichalcogenides (TMDs) at cryogenic temperature and in hBN at room temperature. This work provides deep insights into the electronic, spin, and valley properties of TMDs and hBN. It also paves the way towards the application of 2D vdW materials for quantum optical applications. The materials engineering approaches developed here can be applied to the optimization of other optical and quantum materials.

4:45pm **2D+EM+NS+QS+SS+TF-WeA-11 Macroscopic Tin Monochalcogenide Van Der Waals Ferroics: Growth, Domain Structures, Curie Temperatures and Lateral Heterostructures, Eli Sutter, Peter Sutter, University of Nebraska - Lincoln**

2D and layered van der Waals crystals present opportunities for creating new families of ferroics with switchable electric polarization, elastic strain, or magnetic order at thicknesses down to the single-layer limit. Synthesis, however, typically leads to small crystals with sizes ranging from below 100 nm (e.g., for SnTe ferroelectrics) to a few  $\mu\text{m}$  (e.g., for SnSe ferroelectrics). The limited size and proximity to edges affects the ferroelectric and ferroelastic domain patterns, restricts the experimental methods available to probe emerging properties, and severely limits the ability to fabricate complex device architectures required for accessing functionalities in van der Waals ferroelectrics.

Here, we report the realization of in-plane ferroelectric few-layer crystals of the monochalcogenides tin(II) sulfide and selenide (SnS, SnSe) whose linear dimensions exceed the current state of the art by up to one order of magnitude. Such large crystals allow the investigation of ferroic domain patterns that are unaffected by edges and finite size effects. Analysis of the abundant stripe domains by electron microscopy and nanobeam electron diffraction shows two distinct domain types, twin domains separated by positively charged walls with alternating head-to-head and tail-to-tail polarization as well as not previously observed purely rotational domains connected by neutral domain walls with head-to-tail dipoles. Access to large ultrathin crystals allowed determining the Curie temperatures of few-layer SnSe<sup>1</sup> and SnS van der Waals ferroelectrics.

Finally, we demonstrate the integration of the ultrathin ferroelectric SnSe and SnS into lateral heterostructures.<sup>2</sup> A two-step process produces crystals comprising an SnSe core laterally joined to an SnS edge-band, as confirmed by Raman spectroscopy, electron microscopy imaging, and diffraction. The ability of the lateral interface to direct excited carriers, probed by cathodoluminescence, shows electron transfer over 560 nm diffusion length from the SnS edge-band. The ferroelectric heterostructures adopt two domain configurations, with domains either constrained to the SnSe core or propagating across the entire SnSe-SnS flakes.

The combined results demonstrate industrial scale in-plane ferroelectrics as well as multifunctional van der Waals heterostructures, presenting extraordinary opportunities for manipulating ferroelectric domain patterns and carrier flow.

(1) Sutter, E.; Ghimire, P.; Sutter, P. *J Am Chem Soc* **2024**, *146* (46), 31961-31968. DOI: 10.1021/jacs.4c11558.

(2) Sutter, E.; Ghimire, P.; Sutter, P. *ACS Nano* **2024**, *18* (44), 30829-30837. DOI: 10.1021/acsnano.4c11341.

5:00pm **2D+EM+NS+QS+SS+TF-WeA-12 Machine Learning Analysis of Molecular Beam Epitaxy Growth Conditions, Mingyu Yu, Ryan Trice, Isaiah Moses, Wesley Reinhart, Stephanie Law, Penn State University**

Machine learning models hold the potential to explore parameter space autonomously, quickly establish process-performance relationships, and diagnose material synthesis in real time. This reduces reliance on manual intervention in parameter space exploration, enabling more precise and efficient mechanistic control. For molecular beam epitaxy (MBE), despite its breakthroughs in materials synthesis, its stringent growth conditions and complex epitaxial mechanisms make the process of optimizing growth process time-consuming and expensive. Therefore, leveraging machine learning to develop autonomous MBE growth platforms presents a highly promising prospect. Our study on the multi-modal machine learning-guided MBE synthesis is based on a comprehensive high-quality dataset of GaSe thin films grown on GaAs (111)B substrates. GaSe is an emerging two-dimensional semiconductor material with intriguing properties, including thickness-tunable bandgaps, nonlinear optical behaviors, and intrinsic p-type conductivity. Moreover, as a representative member of the van der Waals (vdW) chalcogenide semiconductor family, insights gained from studying GaSe can be extended to other vdW chalcogenides. In this work, we aim to leverage machine learning to analyze the relationships between

growth conditions (Ga flux, Se:Ga flux ratio, and substrate temperature) and the resulting sample quality, as well as the correlations among various characterization results including in situ RHEED patterns and ex situ x-ray diffraction rocking curve full-width at half maximum (FWHM) and atomic force microscopy (AFM) root mean square (RMS) roughness. Unsupervised learning on RHEED patterns reveals a well-defined boundary between high- and low-quality samples, capturing physically meaningful features. Mutual information analysis shows a strong correlation between RHEED embeddings and rocking curve FWHM, while the correlation with AFM RMS roughness is weak. Among key growth conditions, growth rate most strongly influences FWHM, whereas the Se:Ga flux ratio primarily affects RMS roughness and the RHEED embeddings. Supervised learning models trained to predict FWHM and RMS roughness demonstrate moderate accuracy, with significant improvement achieved by incorporating RHEED embeddings. Furthermore, anomaly detection via residual analysis in supervised learning aligns well with unsupervised classification from RHEED, reinforcing the reliability of the predictive models. This study establishes a data-driven framework for machine learning-assisted MBE, paving the way for real-time process control and accelerated optimization of thin-film synthesis.

5:15pm **2D+EM+NS+QS+SS+TF-WeA-13 Promoting Crystallographic Alignment in SnSe Thin Films using Step Edges on MgO by MBE, Jonathan Chin, Marshall Frye, Joshua Wahl, Kayla Chuong, Georgia Institute of Technology; Mengyi Wang, Derrick Liu, Pennsylvania State University; Mingyu Yu, University of Delaware; Qihua Zhang, Nadire Nayir, Adri van Duin, Maria Hilse, Stephanie Law, Pennsylvania State University; Lauren Garten, Georgia Institute of Technology**

SnSe is a van der Waals material that can be scaled down to two dimensions,<sup>1</sup> making it a promising candidate for nanoelectronics such as field effect transistors (FETs).<sup>2</sup> SnSe in the orthorhombic *Pnma* structure exhibits significant electrical anisotropy where the carrier mobility is 45% higher along the [010] direction than the [001] direction in plane,<sup>3</sup> making it necessary to control the in-plane alignment of 2D films for integration into electronic devices. SnSe has been shown to form planar coverage on (100) MgO,<sup>4</sup> with which it has a 1.4% and 5.5% lattice mismatch along the [010] and [001] directions, respectively. However, despite the distinct axial lattice matches, in-situ reflective high-energy electron diffraction (RHEED) shows no preferential SnSe film alignment for films deposited on uncleaned MgO. Therefore, to promote orientation control, we cleaved and annealed the MgO substrates to produce step edges along the surface to increase the local surface energy, thereby encouraging atomic adsorption and alignment. SnSe thin films were then deposited from individual Sn and Se effusion cells via molecular beam epitaxy (MBE) onto the prepared MgO substrates heated to 280 °C for 1-5 minutes with a 1.35:1.00 Se:Sn flux ratio at a 0.083 Å/s growth rate to track the nucleation and growth of SnSe grains. The phase of the SnSe films was confirmed by Raman spectroscopy, exhibiting the characteristic  $A_g^2$ ,  $B_{3g}$ ,  $A_g^3$ , and  $A_g^4$  phonon modes.<sup>5</sup> In-situ RHEED confirmed the in-plane alignment along the [010] and [001] by RHEED relative to the [100] substrate, matching theory projections made using reactive force field (ReaxFF) simulations. Additionally, atomic force microscopy (AFM) shows SnSe grains nucleating at step edges on MgO, while scanning transmission electron microscopy (STEM) reveals how the aligned SnSe grains propagate laterally off step edges, maintaining crystallographic alignment throughout the film layer. Overall, our results demonstrate that SnSe grains preferentially nucleate along the step edges produced parallel to the [100] edge of the MgO substrates. The alignment of a 2D vdW film facilitated by step edge formation demonstrates how to achieve orientated depositions of similar anisotropic vdW films on a substrate of choice, ultimately facilitating the manufacture of 2D nanoscale electronic devices.

1. Zhang, L.-C. *et al. Sci. Rep.* **6**, 19830 (2016).

2. Chhowalla, M. *et al. Nat. Rev. Mater.* **1**, 1–15 (2016).

3. Zhou, M. *et al. J. Mater. Chem.* **5**, 1247–1254 (2017).

4. Chin, J. R. *et al. Nanoscale* **15**, 9973–9984 (2023).

5. Wu, P. *et al. New J. Phys.* **22**, 083083 (2020).

5:30pm **2D+EM+NS+QS+SS+TF-WeA-14 Synthesis of Millimeter-Scale Single-Crystal  $\alpha$ -MoO<sub>3</sub> Nanosheets on Sapphire, Ryan Spangler, Pennsylvania State University; Thiago Arnaud, Joshua Caldwell, Vanderbilt University; Jon-Paul Maria, Pennsylvania State University**

$\alpha$ -MoO<sub>3</sub> is a van der Waals layered semiconductor with biaxial anisotropy that has recently gained interest as an emerging 2D material with a wide band gap (~3 eV), large work function, and high permittivity. Additionally,  $\alpha$ -

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MoO<sub>3</sub> exhibits extreme anisotropy of the dielectric function, enabling in-plane and out-of-plane elliptic or even hyperbolic behavior at various wavelengths. Therefore,  $\alpha$ -MoO<sub>3</sub> also possesses great potential for nanophotonics through the low-loss and directional propagation of hyperbolic phonon polaritons, which result from the interaction of light with lattice vibrations in highly anisotropic polar materials. However, the lack of single-crystal thin film growth techniques limits further advancement of  $\alpha$ -MoO<sub>3</sub>. In this work, we describe a process for the growth of ultra-large, thin, and atomically smooth single crystals of  $\alpha$ -MoO<sub>3</sub> directly on  $a$ -plane sapphire using an alkali-assisted physical vapor transport method. Important parameters necessary for high-quality growth to be discussed include substrate selection, alkali-to-MoO<sub>3</sub> ratio, and substrate temperature. The growth proceeds through a vapor-liquid-solid (VLS) mechanism enabled by the formation and liquefaction of low-melting point alkali molybdate phases. This growth mode greatly enhances lateral expansion to several millimeters and thicknesses ranging from hundreds of nm down to <5 nm. This is far thinner and more expansive than crystals grown without alkali metal additives, which can exceed several micrometers in thickness while being limited to a few tens of micrometers in lateral dimensions. The thin alkali-assisted sheets exhibit clean step-flow growth without grain boundaries over mm-scale areas as revealed by atomic force microscopy and polarized optical microscopy. Raman spectroscopy and X-ray diffraction indicate the high crystalline quality of the  $\alpha$ -MoO<sub>3</sub> films rivaling that of accessible bulk crystals. We will also investigate the propagation of hyperbolic phonon polaritons using scanning near-field optical microscopy (SNOM) to compare hyperbolic phonon polariton lifetimes to values obtained from exfoliated bulk crystals. We find that this growth technique is suitable for exfoliation-free large-scale single-crystal  $\alpha$ -MoO<sub>3</sub> for nanophotonics and other applications.

5:45pm **2D+EM+NS+QS+SS+TF-WeA-15 Studying the Impacts of Growth Temperature and Seeding Promoters on the Structural and Optoelectronic Properties of ReS<sub>2</sub> Grown by CVD**, *Elycia Wright, Kedar Johnson, Amari Gayle, Robin Rousseau, M.K. Indika Senevirathna, Michael D. Williams*, Clark Atlanta University

Rhenium disulfide (ReS<sub>2</sub>) is a fascinating member of the transition metal dichalcogenide (TMD) family, which has recently gained significant attention due to its distinct distorted octahedral 1T crystal structure characterized by triclinic symmetry. This distinctive structure shows that ReS<sub>2</sub> holds remarkable properties, including anisotropic electronic, optical, and mechanical characteristics. Unlike other TMDs such as MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, and WSe<sub>2</sub>, ReS<sub>2</sub> possesses a band structure that remains consistent regardless of the layer thickness. Due to weak interlayer coupling, it maintains a direct band gap in its bulk and monolayer forms. This unique characteristic makes ReS<sub>2</sub> particularly promising for applications in highly responsive photodetectors. To maximize the potential of ReS<sub>2</sub> for optoelectronic applications, it is essential to address the challenges associated with its anisotropic growth, distorted structure, and weak interlayer interactions. The anisotropic nature of ReS<sub>2</sub> can lead to variations in growth rates in different directions, resulting in multidomain structures that complicate the production of single-crystal ReS<sub>2</sub> on a large scale.

In this study, we will synthesize ReS<sub>2</sub> by chemical vapor deposition (CVD) at various temperatures and utilize seeding promoters to facilitate the growth of single crystals with continuous layers. We will employ advanced techniques such as confocal microscopy, Raman spectroscopy, and photoluminescence spectroscopy to systematically investigate how the growth temperature and seeding promoters affect the structural and optoelectronic properties of ReS<sub>2</sub>.

6:00pm **2D+EM+NS+QS+SS+TF-WeA-16 Growth and Characterization of InSe Thin Films on GaAs(111)B and Si(111)**, *Maria Hilse*, Penn State University

Urgent societal and environmental needs have sparked searches for high-mobility 2D materials with sizeable bandgap and decent stability under ambient conditions for use in ultra-low power, ultra-high performance field effect transistors. With a carrier mobility exceeding 1000 cm<sup>2</sup>/Vs, small electron effective mass, flat electronic band dispersions, excellent optoelectronic, possible ferroelectric properties and a close-to-ideal solar spectrum matched bulk bandgap of 1.26 eV, InSe shows high potential for future use in electronics. Due to the layered nature, and the many members of different polytypes in the InSe materials family, intriguing confinement phenomena and exotic electron-hole coupling mechanisms tunable by the number of single layers add to the potential wealth of properties in InSe.

In this study, InSe thin films were grown by MBE on GaAs(111)B and Si(111). The presence of many InSe phases required a systematic mapping of the growth parameters to identify conditions for single-phase, single-polytype, and single-crystal growth. Through structural characterization in- and ex-situ using reflection high-energy electron and X-ray diffraction, growth conditions for solely gamma-phase, crystalline InSe films were found. Although the structural properties of the films presented nearly unchanged over a small window of growth conditions, the film morphology was seen to sensitively depend on the Se:In flux ratio. Raman spectroscopy confirmed the phase and polytype assignment deduced from large-area structural characterization.

Microstructure analysis, however, revealed a high degree of structural defects in the films. Nano-scale domains of varying single layer stacking sequences, high-angle rotational domains as well as single layers of unusual bonding configuration resulting in a novel InSe polymorph were found in the films. The total number of defects and the general locations of the new polymorph varied in films across GaAs and Si. The highest structural homogeneity was found for InSe films grown on Si.

Density functional theory calculations for a representative selection of the experimentally observed defects confirmed that most defects, including the novel polymorph have formation energies at or below the thermal budget of the MBE synthesis process. Although the bandgaps of all InSe polytypes and polymorphs possess comparable values, large differences were found in their relative offsets. Due to the random distribution of polytypes and polymorphs in the film, our study suggests a high degree of electronic disorder in these films. Electrical transport showed a variable-range hopping-like behavior supporting the hypothesis of electronic disorder.



## 2D Materials

Room 208 W - Session  
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM

### 2D Materials: Optoelectronics and Moire Excitons

Moderator: Daniel Yimam, Oak Ridge National Laboratory

8:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1 Probing the Ultrafast Charge Dynamics and Exciton Emission from Single Atomic Defects in 2D Semiconductors by Lightwave-Driven STM**, *Laric Bobzien, Lysander Huberich, Jonas Allerbeck, Eve Ammerman, Nils Krane, Andres Ortega-Guerrero, Carlo Pignedoli, Oliver Gröning*, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland; *Joshua A. Robinson*, The Pennsylvania State University; *Bruno Schuler*, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland **INVITED** Two-dimensional (2D) semiconductors provide an exciting platform to engineer atomic quantum systems in a robust, yet tunable solid-state system. This talk explores the intriguing physics of single point defects in transition metal dichalcogenide (TMD) monolayers, investigated through atomically resolved scanning probe microscopy.

We have determined the layer-dependent charge transfer lifetimes of selenium vacancies in  $\text{WSe}_2$  on graphene substrates, spanning picosecond to nanosecond timescales [1]. By leveraging our recently developed lightwave-driven scanning tunneling microscope (THz-STM) [2,3], we could probe the ultrafast charge dynamics on the atomic scale. Time-domain sampling with a THz pump-THz probe scheme enabled capturing atomic-scale snapshots of transient Coulomb blockade, a hallmark of charge transport mediated by quantized defect states [4].

Moreover, the extended charge state lifetimes provided by hBN decoupling layers facilitated the local, electrical stimulation of excitonic emission from pristine  $\text{MoS}_2$  and individual charged defects via STM luminescence (STML).

By combining the structural and electronic properties accessible by conventional scanning probe microscopy with the optical fingerprint from STML and the excited-state dynamics revealed through pump-probe THz-STM, we gain a comprehensive microscopic understanding of localized quantum states in low-dimensional materials.

#### References:

- [1] L. Bobzien et al. Phys. Rev. Lett. (accepted, arxiv: 2407.04508)
- [2] J. Allerbeck et al. ACS Photonics 10, 3888 (2023)
- [3] L. Bobzien et al. APL Mater. 12, 051110 (2024)
- [4] J. Allerbeck et al. arXiv:2412.13718 (2024)
- [5] L. Huberich et al. (in preparation)

8:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3 Many-Body Effects on Excitons, Trions, and Defect-Bound States in 2D Materials**, *Kai Xiao, Taegwan Park, Alexander Poretzky*, Oak Ridge National Laboratory, USA; *Xufan Li*, Honda Research Institute; *Kyungnam Kang*, Oak Ridge National Laboratory, USA; *Austin Houston*, University of Tennessee, Knoxville; *Christopher Rouleau, David Geohagan*, Oak Ridge National Laboratory, USA Two-dimensional (2D) materials, particularly transition metal dichalcogenides (TMDs) exhibit strong many-body interactions due to reduced dielectric screening and spatial confinement. These interactions, involving electrons, holes, excitons, phonons, and plasmons, give rise to emergent phenomena distinct from their bulk counterparts. In this talk, I will present our recent investigations into the many-body effects on the optical properties and ultrafast excitonic dynamics of monolayer and bilayer TMDs. Specifically, we synthesized isotopically pure monolayer  $\text{MoS}_2$  and highly defective  $\text{WS}_2$  via nonequilibrium chemical vapor deposition, enabling a controlled study of isotope effects, defects, and background doping on excitonic behavior. Using ultrafast laser spectroscopy and temperature-dependent optical spectroscopy, we observed pronounced many-body interactions, including exciton-phonon and exciton-electron coupling, which significantly influence exciton energy, dynamics, and light-matter interactions in both monolayer and bilayer TMDs. These strong interactions give rise to novel quantum states and make 2D materials promising platforms for next-generation optoelectronics, quantum information technologies, and fundamental condensed matter physics.

Synthesis science was supported by the U.S. Dept. of Energy, Office of Science, Materials Science and Engineering Division. This work was performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

8:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4 Proximity-Induced "Magic" Raman Bands in TERS Spectra of  $\text{MoS}_2$  /  $\text{WS}_2$  @ 1L h-BN-Capped Gold**, *Andrey Krayev*, HORIBA Scientific; *Pavel Valencia Acuna*, PNNL; *Ju-Hyun Jung*, Pohang University of Science and Technology (POSTECH), Republic of Korea; *Cheol-Joo Kim*, POSTECH, Republic of Korea; *Andrew Mannix*, Stanford University; *Eleonora Isotta*, Max Planck Institute for Sustainable Materials, Germany; *Chih-Feng Wang*, PNNL

Recently it was proposed to use the monolayer h-BN – capped gold substrates as an ideal platform for the gap mode TERS and TEPL imaging, that on the one hand, should preserve strong gap mode enhancement of Raman signal due to small thickness (0.3 nm) of the dielectric h-BN layer, and on the other hand preserve strong TEPL response due to de-coupling of 2D semiconductors from the metallic substrate. TERS data collected on mono- and a few-layer-thick crystals of  $\text{MoS}_2$  and  $\text{WS}_2$  on 1L-h-BN-capped gold show both the TERS and TEPL response, confirming the validity of the proposed approach.

In addition to the enhancement of both the PL and Raman signal, in the course of assessment of TERS/TEPL response of mono- and a few-layer-thick crystals of  $\text{MoS}_2$  and  $\text{WS}_2$  deposited on 1L h-BN-capped gold we observed in TERS spectra, completely unexpectedly, appearance of Raman bands at about  $796\text{ cm}^{-1}$  and  $76\text{ cm}^{-1}$  which are not normally observed in regular Raman spectra of h-BN or  $\text{WS}_2/\text{MoS}_2$ . We can safely state that these "magic" bands belong to h-BN as they appear at the same spectral position in TERS spectra of both the monolayer  $\text{MoS}_2$  and  $\text{WS}_2$  deposited on the monolayer h-BN capped gold, moreover, the  $796\text{ cm}^{-1}$  band often was the strongest band observed in TERS spectra, even stronger than A' mode from  $\text{WS}_2$  or  $\text{MoS}_2$ . Presence of the transition metal dichalcogenide (TMD) monolayer is mandatory for the appearance of these "magic" bands as they are absent outside of the monolayer TMDs in these samples. Literature search showed that similar (but not identical) phenomenon was observed earlier in h-BN encapsulated  $\text{WSe}_2/\text{MoSe}_2$  and  $\text{WS}_2$ . There have been several significant differences between our data and the earlier reported one: in our case we have not been able to observe the "magic bands" in  $\text{MoSe}_2$  and  $\text{WSe}_2$  @ 1L h-BN@Au, while  $\text{WS}_2$  monolayers deposited on the same substrate as  $\text{WSe}_2$ , showed expected response. More importantly, the excitation laser wavelength dependence in our case was completely different from what was reported earlier: in  $\text{WS}_2$ -based samples we observed strong "magic" bands with excitation at 830 nm, 785nm, 594nm, but not 633nm, the wavelength closest to the A exciton in this material. This excitation profile is remarkably reminiscent of the excitation profile of the monolayer  $\text{WS}_2$  in intimate contact with silver where we observed strong dip of the intensity of main A' mode in TERS spectra at 633nm excitation wavelength.

We will argue that intricate interaction between the tip-substrate gap plasmon, TMD excitons and most probably, normally mid-IR-active phonons in h-BN is responsible for the appearance of observed "magic" bands.

9:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-5 Correlated Excitons in TMDC Moiré Superlattice**, *Sufei Shi*, Carnegie Mellon University **INVITED**

In a strongly correlated electronic system, Coulomb interactions among electrons dominate over kinetic energy. Recently, two-dimensional (2D) moiré superlattices of van der Waals materials have emerged as a promising platform to study correlated physics and exotic quantum phases in 2D. In transition metal dichalcogenides (TMDCs) based moiré superlattices, the combination of large effective mass and strong moiré coupling renders the easier formation of flat bands and stronger electronic correlation, compared with graphene moiré superlattices. Meanwhile, the strong Coulomb interaction in 2D also leads to tightly bound excitons with large binding energy in TMDCs. In this talk, we will discuss how to use optical spectroscopy to investigate excitonic physics and strongly correlated phenomena in TMDC moiré superlattice, along with correlated exciton states arising from strong interactions.

9:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-7 Sub-Stoichiometric Phases in 2D  $\text{MoTe}_2$** , *Onyedikachi Alanwoko, Nirasha Rajapakse, Matthias Batzill*, University of South Florida

Atom vacancy formation in crystalline materials is energetically expensive. To lower the energy cost for non-stoichiometry, point defects can condense into energetically more favorable extended defects. Studies on Mo-dichalcogenides have shown that excess Mo is condensed into closed, triangular Mirror Twin Boundary (MTB) loops. These MTBs can form in high densities where the triangular loops connect and form a cross-hatched network of MTBs. Here we show through Scanning Tunneling Microscopy (STM) that periodically ordered MTB networks can obtain a homologous series of sub-stoichiometric  $\text{MoTe}_{2-x}$  phases. We systematically investigate

the preparation conditions (which include a variation of the growth temperature, Te-desorption by post-growth annealing, and vapor-deposited Mo), enabling the controlled synthesis of these new phases. The different phases require different synthesis procedures, and once formed, these phases appear thermally stable in vacuum. The ability to control and create these different phases of MoTe<sub>2</sub> and other two-dimensional (2D) materials is a promising way of realizing new electronic and chemical properties of 2D materials. Particularly promising is the observation that we can react MoTe<sub>2</sub> with dissimilar transition metals to create new doped or alloyed 2D materials with potentially desirable properties.

**11:00am 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-13 Microwave Imaging of Excitonic States and Fractional Chern Insulators in 2D Transition Metal Dichalcogenides, Zhurun Ji, SLAC National Accelerator Laboratory/ MIT INVITED**

Nanoscale electrodynamics offers a unique perspective on states with bulk-edge correspondence or spatially dependent excitations. I will introduce our latest advancements in optically coupled microwave impedance microscopy, a technique that enhances our capability to explore electrodynamics at the nanometer scale. I will discuss our recent studies utilizing this technology to extract spectroscopic information on exciton excitations within transition metal dichalcogenide systems. Additionally, I will share our recent findings on probing topological and correlated electronic states, specifically the fractional Chern insulator states in twisted TMD bilayers.

**11:30am 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-15 Control and Properties of Single Dislocations in Van Der Waals Nanowires, Peter Sutter, Eli Sutter, University of Nebraska - Lincoln**

Line defects (dislocations) not only govern the mechanical properties of crystalline solids but they can also produce distinct electronic, thermal, and topological effects. Identifying and accessing this functionality requires control over the placement and geometry of single dislocations embedded in a small host volume to maximize emerging effects. We have identified a synthetic route that enables the rational placement and tuning of dislocation in van der Waals nanowires, where the 2D/layered crystal structure limits the possible defect configurations and the nanowire architecture puts single dislocations in close proximity to the entire host volume.<sup>1</sup> While homogeneous layered nanowires carry individual screw dislocations, the synthesis of radial (core-shell) nanowire heterostructures transforms the defect into a mixed (helical) dislocation whose edge-to-screw ratio is continuously tunable via the core-shell lattice mismatch.

Such deterministic control over defects now enables the probing of functionality arising with single dislocations. For example, germanium sulfide van der Waals nanowires carrying single screw dislocations incorporate Eshelby twist and thus adopt a chiral twisted structure,<sup>2</sup> which for the first time allowed the identification of chirality effects in the photonic properties of a single nanostructure.<sup>3</sup> Using cathodoluminescence spectroscopy, whispering gallery modes could be excited and probed to directly compare the photonics of chiral and achiral segments in single nanowires. The data show systematic shifts in energy, which with the help of simulations are assigned to chiral whispering gallery modes in wires hosting a single dislocation.

The ability to design nanomaterials containing individual dislocations with controlled geometry paves the way for identifying a broad range of functional properties of dislocations, with the potential to herald a paradigm shift from the traditional strategy of suppressing dislocations to embracing and harnessing them as core elements of new technologies.

1. P. Sutter, R.R. Unocic, and E. Sutter, *Journal of the American Chemical Society* 145, 20503 (2023); DOI: 10.1021/jacs.3c06469
2. P. Sutter, S. Wimer, and E. Sutter, *Nature* 570, 354 (2019); DOI: 10.1038/s41586-019-1147-x
3. P. Sutter, L. Khosravi-Khorashad, C.V. Ciobanu, and E. Sutter, *Materials Horizons* 10, 3830 (2023); DOI: 10.1039/D3MH00693J

**11:45am 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-16 Two-Dimensional Keldysh Theory for Non-Resonant Strong-Field Ionization of Monolayer 2D Materials, Tsing-Hua Her, UNC Charlotte; Che-Hao Chang, NTHU, Taiwan; Kenan Darden, UNC Charlotte; Tsun-Hsu Chang, NTHU, Taiwan; Hsin-Yu Yao, NCCU, Taiwan**

Over the past decade, a diverse array of intense light interactions with monolayer two-dimensional (2D) materials have been reported, including low- and high-order harmonic generation (HHG), multiphoton absorption, optical injection of spin and charge currents, terahertz generation, and

laser-induced dielectric breakdown. These processes are all initiated by interband transition of electrons induced by light with photon energy smaller than the bandgap energy. Some modeling efforts based on perturbation theory were attempted but their discrepancies with experiments are at least one order of magnitude, highlighting the lack of theoretical understanding of strong-field ionization in monolayer 2D materials. In this work, we report a new formalism of strong-field ionization for monolayer two-dimensional semiconductors based on 2D Keldysh (KLD) theory [T. -H. Her et al., *Optica* 12, 538-545 (2025)]. We take this approach because the original Keldysh theory [L. V. Keldysh, *Soviet Physics JETP* 20, 8 (1965)] is the only theory that yields, for simplified band dispersion, analytical formulas for the cycle-averaged non-resonant ionization rate in bulk solids induced by a monochromatic electric field of arbitrary strength. It provides a smooth transition between multiphoton and tunneling ionization as what we now call the ‘Keldysh parameter’,  $\gamma$ , varies from  $\gamma \gg 1$  to  $\gamma \ll 1$ . Due to their analyticity, Keldysh’s formulas are widely employed for qualitative modeling of strong-field ionization in bulk solids. In this presentation, we generalize Keldysh’s formulas to monolayer two-dimensional semiconductors. We derive closed-form formulas and their asymptotic forms for a two-band model with a Kane dispersion. We also derive selection rules related to the parity of multiphoton orders near the band edge. We validate our theory by comparing it to recent experiments and modeling of strong-field ionization in monolayer transition metal dichalcogenides (TMDs) with very good agreement (Figs. 1-3 of supplemental document) Specifically, our theory predicts a higher interband electron tunneling rate for 2D compared to 3D in the MIR frequency range, which successfully explains the 10x discrepancy (Fig. 3) between the experiment and modeling for HHG from monolayer TMDs [Liu et al., *Nature Phys* 13, 262–265 (2017)]. Considering the tremendous success of the original Keldysh theory in describing strong-field optical phenomena in atoms and solids, our 2D Keldysh theory is expected to find a wide range of applications in intense light-2D material interaction, such as optical limiting, multi-photon photodetection, THz generation through quantum interference, and photo-carrier doping for HHG.

**12:00pm 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-17 Thickness Dependent Band Gap and Electrical Anisotropy of 2DSnSe, Marshall Frye, Jonathan Chin, Joshua Wahl, Jeremy Knight, Georgia Institute of Technology; Walter Smith, Purdue University; Dilara Sen, Samuel Kovach, Kenyon University; Frank Peiris, Kenyon College; Charles Paillard, University of Arkansas; Thomas Beechem, Purdue University; Anna Osterholm, Lauren Garten, Georgia Institute of Technology**

2D SnSe presents unique opportunities for optoelectronics, and scalable microelectronics, but it is first critical to understand how the electrical and optical response change upon downscaling. Tailoring the band gap and electrical anisotropy of 2D monochalcogenides, like SnSe, has previously been shown but the mechanisms that drive the changes in band gap are still not understood. This study reveals how changes in bond length and structure drive the thickness dependences of band gap, carrier mobility and lifetime of SnSe thin films. Molecular beam epitaxy is used to deposit (2h00) oriented SnSe thin films with thicknesses ranging from 4 nm to 80 nm. The direct band gap increases from 1.4 eV at 80 nm to 1.9 eV at 4 nm, underscoring the potential of SnSe as a tunable and direct band gap material for thin film optoelectronics. Raman spectroscopy shows different simultaneously changes in the crystal structure and bonding occurring parallel versus perpendicular to the 2D plane with decreasing film thickness. TEM further supports the hypothesis that the increase in the band gap with reduced thickness is due to changes in crystal structure resulting in a contraction of the out-of-plane SnSe covalent bonds, while the in-plane bond length increases. In addition to the reduction in band gap, tracking the time dependent photoluminescence shows an increase in carrier lifetime with decreasing film thickness, while Hall measurements show a change in the carrier mobility with decreasing thickness. Overall, this work provides the critical missing insight needed to design these optically and electronically relevant 2D materials for scalability.

# Thursday Afternoon, September 25, 2025

## 2D Materials

### Room 208 W - Session 2D+AQS+MI+NS+QS+TF-ThA

#### 2D Materials: Magnets and Topological Phenomena

Moderators: Rafik Addou, The University of Texas at Dallas, Zhurun Ji, MIT

#### 2:15pm 2D+AQS+MI+NS+QS+TF-ThA-1 Non-Local Transport from Magnetic Topological Superconductivity in 2D Fe-Chalcogenides, *Kenneth Burch*, Boston College INVITED

Magneto-Chiral topological superconductivity is a rare phase long pursued for error-free quantum computation. Its 1D chiral modes possess topologically protected long-range coherence well beyond that of the Cooper pairs, which could be fruitful for quantum transduction and low-temperature spin transport. While evidence for such modes is mounting, unambiguous signatures, such as non-local transport via co-tunneling, remain elusive. I will describe our realization of 1D chiral hinge modes mediating the direct tunneling of electrons from source to drain in FeTe<sub>0.55</sub>Se<sub>0.45</sub>. Specifically, I will discuss our evidence that the non-local tunneling signatures are decoherence-free and emerge from this material's combination of surface magnetism, bulk topology, and superconductivity. Time remaining, I will discuss how these advances can be used for Majorana Circuits and future efforts in cryogenic spintronics

#### 2:45pm 2D+AQS+MI+NS+QS+TF-ThA-3 Integer and Fractional Chern Insulators in moiré MoTe<sub>2</sub>, *Yihang Zeng*, Purdue University INVITED

The fractional Chern insulator (FCI), a lattice analogue of the renowned fractional quantum Hall state, was theorized to exist without external magnetic field. FCI provides a pathway towards novel topologically ordered quantum phases that are useful for decoherence-free quantum computation. Two-dimensional (2D) moiré materials, featuring strong correlation, non-trivial band topology and unparalleled tunability, stands as an ideal platform for realizing FCI. In this talk, I will first present our innovative optoelectronic detection method, which is capable of detecting the chemical potential in arbitrary 2D materials. Employing this new technique, we successfully observed an FCI and integer Chern insulator in the zero magnetic field limit in MoTe<sub>2</sub>-based moiré materials. We further study the FCI and ferromagnetism as a function of twist angle.

#### 3:15pm 2D+AQS+MI+NS+QS+TF-ThA-5 Conducting Scanned Probe Investigations of the Bismuthine Termination of Intrinsic Topological Superlattice Bi<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub>, *Lakshan Don Manuwelge Don, Mysidia Leff, Md. Sakauat Hasan Sakib, Miami University; Seth Shields, The Ohio State University; Joseph Corbett, Miami University*

Topological materials, characterized by symmetry-protected electronic states and robust surface conduction, represent a frontier in quantum materials research. Their non-trivial band topology enables dissipationless edge states, spin-momentum locking, and resilience to disorder, making them strong candidates for spin-orbit torque devices, magnetic field sensors, and polarized light detectors, to name a few. These properties have positioned topological materials as important material of interest as development of scalable quantum technologies grows.

In this study, we explore the atomic and electronic properties of the bismuthine-terminated topological semimetal Bi<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub> using scanning tunneling microscopy (STM) and conductive atomic force microscopy (C-AFM). Bi<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub> is an intrinsic superlattice material s comprised of a Bi<sub>2</sub>Se<sub>3</sub> quintuple layer (QL) slab and a 2D Bismuthine (Bi<sub>2</sub>) layer separated by a van der Waals gaps. The topological surface state on the 001 orientation depends on the terminating layer, with two distinct possible topologically protected surface states.

The unique step heights between the Bi<sub>2</sub>Se<sub>3</sub> QL and Bismuthine layer enable termination characterization through careful step height analysis. Atomically resolved STM measurements on a Bismuthine terminated step reveal a distinct honeycomb lattice, while scanning tunneling spectroscopy (STS) captures a Dirac cone in local density of states centered at the Fermi level, in excellent agreement with angle-resolved photoemission spectroscopy (ARPES).

Using C-AFM under ambient conditions, we investigate force-dependent I-V spectroscopy. Utilizing step height analysis, we find a bismuthine terminated step and perform point spectroscopy. At low applied forces, differential conductance (dI/dV) spectra reveal a Dirac cone, mirroring STM results and confirming the presence of topologically protected surface states even under ambient conditions! As mechanical force increases, we observe a transition in transport behavior, from quantum tunneling to Ohmic conduction. Additionally, a voltage and force-dependent crossover from direct tunneling to Fowler-Nordheim tunneling is identified.

Our findings revealing the atomic structure and Dirac cone of the bismuthine termination in the topological semimetal Bi<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub>. Interestingly these feature are observable even under ambient condition. We find no degradation with time, freshly grown sample versus those that have sat for months give the same results.

#### 3:30pm 2D+AQS+MI+NS+QS+TF-ThA-6 Local Spectroscopy Study of Gate-controlled Energy Gap in Monolayer 1T'-WTe<sub>2</sub>, *Tiancong Zhu*, Purdue University; *Zehao He*, University of California at Berkeley; *Michal Papaj*, University of Houston; *Samuel Stolz*, Department of Physics, University of California, Berkeley; *Tianye Wang, Canxun Zhang, Yan-Qi Wang, Joel Moore, Zi Qiang Qiu, Feng Wang, Michael Crommie*, University of California at Berkeley

The interplay between strong correlation and topology can lead to intriguing quantum phases of matter. In monolayer 1T'-WTe<sub>2</sub>, the non-trivial topology gives rise to the quantum spin Hall insulator (QSHI) phase, characterized by helical 1D edge states surrounding the insulating 2D bulk. While experimental evidences support quantized conductance through the 1D helical edge states, the nature of the insulating bulk, whether attributed to spin-orbit coupling or strong correlation, remains under debate. Here, we employ scanning tunneling microscopy and spectroscopy (STM/S) on gate-tunable 1T'-WTe<sub>2</sub> devices to shed light on this problem. Our samples are fabricated using a combination of molecular beam epitaxy (MBE) and van der Waals (vdW) stacking technique, which allows us to synthesize high-quality monolayer 1T'-WTe<sub>2</sub> films on a gate tunable graphene field effective transistor supported by hBN. Gate-dependent STS reveals a substantial energy gap in 1T'-WTe<sub>2</sub> at its charge neutrality, which diminishes when the Fermi level is tuned into either the conduction or valence band. STS across the sample edges shows that the edge states persist at all gate voltages, while Fourier transform-STM measurement in the bulk further shows the evolution of the bulk band structure at different carrier densities. We will compare our experimental data with existing theoretical models, such as the SOC-induced gap and the proposed excitonic insulator phase, and suggest future experimental directions to further elucidate the origin of the energy gap.

#### 3:45pm 2D+AQS+MI+NS+QS+TF-ThA-7 Exploring Moiré Magnetism in Twisted Two-Dimensional Magnets, *Liuyan Zhao*, University of Michigan INVITED

Moiré superlattice emerges from the interference between two mismatched atomic lattices, and it has led to tremendous success in designing and tailoring the electronic states in two-dimensional (2D) homo- and hetero-structures. Yet, the power of moiré superlattice in controlling the spin degree of freedom and thus modifying the magnetic states is much less explored. Only very recently after the development of 2D magnet research, there have been a few experimental attempts in realizing moiré magnetism in twisted 2D magnet homo-structures. In this talk, I will show our recent effort in studying magnetic phases in twisted double bilayer chromium triiodide (CrI<sub>3</sub>) and progressive steps towards realizing moiré magnetism. Noting that bilayer CrI<sub>3</sub> is a layered antiferromagnet and that any homogeneous stacking of two bilayers necessarily produces zero magnetization, we have revealed, in twisted double bilayer CrI<sub>3</sub>, an unexpected net magnetization showing up at intermediate twist angles and its accompanied noncollinear spin textures. I will show the optical spectroscopy signatures of this twist-induced magnetic phase, then discuss its dependence on twist angle, external magnetic field, and temperature.

## Quantum Science and Technology Mini-Symposium Room Ballroom BC - Session QS-ThP

### Quantum Science and Technology Mini-Symposium Poster Session

**QS-ThP-1 Frugal Quantum Magnetometry for Education, John Muth, Jonathan Rabe**, North Carolina State University

The use of color centers for magnetometry is well established, with the nitrogen-vacancy (NV) center in diamond being the most prominent example. Recently, there has been growing interest in using silicon carbide as a more cost-effective alternative material. However, for educational purposes, the cost of associated optics and electronics can present a significant barrier with many approaches costing in excess of \$10,000.

This poster presents the design of a printed circuit board using off-the-shelf electrical components, integrated with an adjustable 3D-printed optical mount. The entire system can be built for under \$500 (excluding the cost of the diamond). The stand-alone device is compact and portable, and can be connected to a laptop for data acquisition and analysis.

Collected data demonstrate that the system achieves sensitivity in the low microtesla range and that hyperfine splitting can be observed. It can be used to generate color maps that visualize Zeeman splitting and to investigate how the orientation of NV centers affects the fitting of the zero-field splitting. As an alternative to optically detected magnetic resonance (ODMR) in diamond, the use of spin-dependent recombination to enable an all-electrical quantum magnetometer based on silicon carbide will also be briefly discussed.

**QS-ThP-4 Telecom Quantum Photonics Enabled by Erbium-Doped SiC Nanostructures: A Scalable Nanofabrication and Materials Science Engineering Approach, Alexander Kaloyeros<sup>1</sup>, Spyros Galis**, University at Albany-SUNY

The development of scalable photonic technologies relies on integrating compact, on-chip nanoscale devices into quantum photonic integrated circuits (qPICs). Key components of these systems, such as quantum LEDs (qLEDs) that are based on engineered point-defect nanoscale emitters, require material platforms that support operation at elevated temperatures, enable electrical addressability, and are compatible with high-yield, large-scale fabrication. Additionally, operation in the highly desirable telecom C-band (~1540 nm) is critical for low-loss optical communication. However, despite significant progress, none of the current material systems has been able to meet all these requirements within this important set of constraints. Current technologies are limited by non-ideal emission wavelengths, low-yield fabrication of emitters (e.g., randomness in spatial placement, orientation, and emission frequency), and the need for cryogenic temperatures. Collectively, these challenges pose major barriers to scalable integration. We present a nanofabrication- and materials-engineering-driven strategy to create a material platform that resolves these key challenges. Notably, this platform enables coherent optical control at 77 K, including the ability to resolve Rabi oscillations from a single  $\text{Er}^{3+}$  emitter, which emit in the telecom C-band (~1534 nm), and narrow optical linewidth of ~90 MHz. The approach is based on the fabrication of arrays of  $\text{Er}^{3+}$ -doped silicon carbide (SiC) hollow nanopillars (HNPs) and nanowires (NWs) using a scalable, CMOS-compatible process. A key breakthrough is the precise spatial positioning of  $\text{Er}^{3+}$  ions with sub-5 nm accuracy. This is achieved through a novel strategy in which placement is governed not by lithographic patterning but by the critical dimension of the nanostructures, defined by our highly controlled conformal SiC deposition. This addresses one of the primary limitations of current single-photon emitter platforms: the randomness in emitter location, orientation, and spectral properties that impedes large-scale integration. The fabrication of these foundational structures and their properties will be presented in the context of advancing quantum photonic integrated devices. Furthermore, we demonstrate the ability to control both the density and spatial distribution of Er ions, enabling the isolation of single and few  $\text{Er}^{3+}$  ions at temperatures  $\geq 77$  K—capabilities not previously achievable in bulk systems. Together with polarization control and compatibility with optical cavity integration, these results highlight the potential of this platform for scalable, high-performance quantum photonic technologies.

**QS-ThP-5 Accurate Atomic Correlation and Total Energies for Correlation Consistent Effective Core Potentials (ccECP) for Transition Metals, Aqsa Shaikh**, North Carolina State University, India

In this work we utilize the correlation consistent effective core potentials (ccECPs) and present highly accurate correlation and total energy calculations for a selected set of transition metals and other heavy elements. We calculated the total energies using a variety of sophisticated correlated methods including configuration interaction (CI), coupled-cluster (CC) to multiple excitations and also with stochastic sampling approaches such as Quantum Monte Carlo (QMC). Calculations were performed with basis sets up to cc-pV5Z to limit discrepancies and then extrapolated to estimate the complete basis set limit. Kinetic energies were similarly assessed through CI to various excitation levels. We also present diffusion Monte Carlo (DMC) energies, providing insight into fixed-node/phase biases in single-reference trial wave functions. These results establish reliable benchmarks for ccECP performance across a broad spectrum of electronic structure methods, ensuring their utility in future high-accuracy calculations in correlated deterministic and stochastic frameworks.

**QS-ThP-6 Optimization of DC Magnetron Sputtering Process for Coherent Nb-based Superconducting Quantum Electronics, Kiana Reed, Joseph Falvo, Marcelo Velasco-Forest, Ivan Lainez, Kasra Sardashti**, Laboratory for Physical Sciences

Niobium (Nb) is a widely used superconducting material in thin-film form for quantum and superconducting electronic applications. In this work, we develop a robust Nb sputtering process optimized for evaluating candidate substrates for superconducting qubits. Thin Nb films were deposited on Si (001) substrates using direct current (DC) magnetron sputtering under varying powers and deposition times. Initial process optimization was guided by DC transport measurements, including critical temperature, critical field, and residual resistance ratio. Promising recipes were further assessed by fabricating Nb/Si coplanar waveguide resonators and measuring their internal quality factors at microwave frequencies. To mitigate dielectric losses at the metal-substrate interface, we implemented surface cleaning methods such as ex-situ HF etching (solution and vapor) and in-situ argon ion milling. Film morphology and interface quality were characterized using atomic force microscopy and scanning electron microscopy. Building on the optimized deposition parameters, we outline a pathway for screening alternative qubit-compatible substrates, including sapphire and silicon carbide.

**QS-ThP-7 Tunable Superconducting Properties in Mesoscopic SNS Island Arrays, Shiva Dahal, Winston-Salem State University; Bernadeta Srijanto, Oak Ridge National Laboratory; Kasra Sardashti, University of Maryland College Park; John Yi, Winston-Salem State University**

Superconductor array islands offer a uniquely tunable platform for probing fundamental quantum phenomena and advancing next-generation technologies. By precisely controlling Josephson coupling, charging energy, and disorder, these mesoscopic superconductor-normal-metal-superconductor (SNS) arrays enable direct exploration of key quantum phase transitions, including the superconducting-insulating transition and Berezinskii-Kosterlitz-Thouless (BKT) physics. Using advanced lithographic techniques, we pattern superconducting (Nb or Al) islands on thin metal films (Pt, Fe, Co, Ni, and Au) to investigate how geometry, size, spacing, and arrangement affect superconducting, resistive, and magnetic properties, including the critical temperature. Variations in island spacing and film thickness, combined with the use of metals with distinct electronic characteristics, are designed to uncover new strategies for controlling superconductivity and engineering high-performance heterostructures. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) verify fabrication accuracy, surface morphology, and dimensional precision, with observed uniformity and sharp edge definition expected to minimize scattering centers and defects, thereby preserving coherence and enhancing proximity-induced superconductivity. Resistivity measurements will probe the proximity effect, while magnetic characterization under applied fields will reveal flux dynamics and vortex behavior. The use of different metal films with varying electronic and transport characteristics is expected to yield novel material innovations. Overall, this research seeks to develop new strategies for controlling superconductivity, providing valuable insights into the design and fabrication of high-temperature superconductors and quantum devices. By combining precision nanofabrication, systematic materials variation, and rigorous transport and magnetic characterization, this work bridges fundamental condensed-matter physics with practical quantum device engineering, driving both scientific discovery and technological innovation.

## **QS-ThP-8 Probing the Functional Efficacy of Tunable SSWM Microring Resonators as Couplers for Tri-State Entanglement in Photonic Quantum Processors, *Arsh Jha*, North Carolina Central University**

Quantum photonic processors offer major advantages over classical computing through massive parallelism. Conventional two-photon couplers, however, are limited in scalability and flexibility. We present a photonic quantum circuit architecture using a Spontaneous Six-Wave Mixing (SSWM) microring resonator, adapted from classical photonics, as an active logic element generating triphoton entanglement. These three-photon interactions reduce coupler requirements and enable more qubits (greater integration density), hence allowing for greater computational power.

Decoupling allows qubits to temporarily store quantum information without unwanted interactions. Using MEEP simulations, the decoupled state was achieved by sweeping the ring index  $n_{\text{ring}}$  (semiconductor-compatible refractive index tuning) from 2.05 to 2.20 with the bus waveguide fixed at 2.05, until no light propagated into the ring. Coupling coefficients decreased from 0.1094 to 0.0200 (showing detuning) while the Q-factor remained stable (335.9 to 433.38), confirming robust functionality. Coupling spectra retained their shapes with only amplitude reductions, indicating unchanged behavior.

Photon state integrity was evaluated using a custom QuTiP-based photon-photon interaction model, with three modes of four photons each evolving under a Hamiltonian derived from the kappa interaction matrix. For both states, photon purity remained near 1, fidelity averaged  $0.9 \pm 0.1$ , and entropy stayed close to zero. Wigner function analysis showed minimal but consistent state differences, with their time-dependent rotation revealing precise windows for targeted control.

To measure circuit-level performance, a custom quantum photonic architecture was created: three data qubits underwent five different protocol classes i.e. teleportation, simple squeezing, etc. They operated under realistic noise channels with ancilla-assisted measurement. Kappa matrices ( $\kappa$ ) determined entanglement strengths and were swept over time from  $[0, \kappa_{\text{max}}]$  to simulate detuning. This was compared to the control without kappa to determine if detuning affected circuit performance.

Metrics showed that the tunable SSWM microring resonator demonstrates strong potential in quantum photonic circuits with 4/5 protocols receiving better or consistent performance with (bi-state) detuning. Its protocol-dependent performance highlights opportunities for targeted applications, and future work will focus on simulation denoising and broader frequency sweeps to ensure robust, energy-efficient operation.

## **QS-ThP-9 Stability of Entanglement States in (A)Symmetric InAs/GaAs Double Quantum Dots, *Patrick Flanigan, Igor Filikhin, Branislav Vlahovic*, North Carolina Central University**

Double quantum dots (DQDs) are systems where two quantum dots (QDs) are placed close enough together that a single electron will be coupled to both, potentially leading to delocalized states where its position expectation value is outside of the QDs themselves. The individual QDs can have different shapes, sizes, and material compositions, which in turn leads to differing energy level spectra. In a DQD system, the energy levels of a single electron will be a function of both. This makes the DQD a very promising tool for applications such as biochemical sensors and quantum computing. Of particular interest is the case where the QDs are nearly identical, but not exactly. In a real-world device, this kind of asymmetry is inevitable when considering the inherent limits of nano-scale fabrication technology. If DQD systems are to be employed as qubits or sensors, the role that this plays on their properties is critically important — this fabrication-induced surface coarseness can be the catalyst for turning a symmetric DQD into an asymmetric one, and thus will limit the DQD's usefulness in a working device. Here, we present results from 3D computational simulations of a DQD system that has been slightly shifted away from perfect symmetry to better understand the role that this effect plays on the electron's energy level spectrum, available eigenstates, and degree of localization. It was found that even minuscule deviations from total symmetry can cause an electron to transfer from a delocalized state to a localized one. The possibility of rectifying this effect through the use of an applied electric field was also considered.

Figure 1 shows that taking a symmetric pair and changing one of the semi-major axes by a tiny fraction (from 19 to 18.75 nm) causes strong localization. Figure 2 shows that applying an electric field will alter the probability ( $P$ ) of finding the electron in the left/right QD's ground state in an asymmetric DQD system; however, a perfect 50-50 split is still not possible.

## 2D Materials

Room 208 W - Session 2D+AQS+EM+NS+QS+TF-FrM

## 2D Materials: Devices and Applications

Moderator: Kai Xiao, Oak Ridge National Laboratory

8:15am **2D+AQS+EM+NS+QS+TF-FrM-1 Charge Transport in Printed Films of Two-Dimensional Materials for Printed and Wearable Electronics, Felice Torrisi**, Imperial College London, UK **INVITED**

Printed electronics has emerged as a pathway for large scale, flexible, and wearable devices[1], Internet-of-Things[2] and smart textiles[3]. Graphene and related two-dimensional (2D) materials offer an ideal platform of novel materials for high performance printed electronics [4,5]. Electronic inks from 2D materials with different electronic properties have been developed to print the different elements of a device: semiconducting or semimetallic inks in the active layer, insulating inks for dielectrics, and conducting inks for electrodes[6].

In this talk I will describe the charge transport mechanisms of surfactant- and solvent-free inkjet-printed thin-film devices of representative few-layer graphene (semi-metal), molybdenum disulphide (MoS<sub>2</sub>, semiconductor) and titanium carbide MXene (Ti<sub>3</sub>C<sub>2</sub>, metal) by investigating the temperature, gate and magnetic field dependencies of their electrical conductivity.[7]

Charge transport in printed few-layer MXene and MoS<sub>2</sub> devices is dominated by the intrinsic transport mechanism of the constituent flakes. On the other hand, charge transport in printed few-layer graphene devices is dominated by the transport mechanism between different flakes.[7]

[1] Torrisi, F. & Carey, T. "Graphene, related twodimensional crystals and hybrid systems for printed and wearable electronics" Nano Today 23, 73 (2018).

[2] C. Scholten et al. "Advanced Technologies for Industry – Product Watch: Flexible and printed electronics", doi: 10.2826/29513 (2021).

[3] Carey, T. et al. "Fully inkjet-printed two-dimensional material field-effect heterojunctions for wearable and textile Electronics" Nat. Commun. 8, 1202 (2017).

[4] Torrisi, F. et al. Inkjet-printed graphene electronics. ACS Nano 6, 2992(3006 (2012).

[5] F. Torrisi & T. Carey "Printing 2D Materials" in "Flexible Carbon-based Electronics" Editors P. Samori and V. Palermo, Ed.: Wiley-VCH, Weinheim, Germany, 2018. ISBN: 978-3-527-34191-7.

[6] D. Akinwande "Two-dimensional materials: printing functional atomic layers" Nat. Nanotechnol. 12, 287 (2017).

[7] E. Piatti, A. Arbab et al. "Charge transport mechanisms in inkjet-printed thin-film transistors based on two-dimensional materials" Nature Electronics 4, 893 – 905 (2021).

8:45am **2D+AQS+EM+NS+QS+TF-FrM-3 Antimony as a Contact Material for Two-Dimensional Semiconductors: Interface Chemistry and Thermal Stability, Fernando Quintero Borbon, Joy Roy, Robert Wallace, Rafik Addou**, University of Texas at Dallas

Antimony (Sb), a semimetal, has emerged as a promising contact material for two-dimensional (2D) semiconductors. Sb contacts have been shown to achieve ultra-low contact barriers. The formation of a Sb–Se bond has been demonstrated as an effective doping strategy in n- and p-FETs with a single WSe<sub>2</sub> channel through Sb-Pt contact modification. These findings underscore the necessity for further investigation into the interface chemistry and thermal stability of Sb on transition metal dichalcogenides (TMDs), to determine whether the interaction remains van der Waals or becomes chemically reactive upon thermal processing.

The present study offers a comprehensive study of the interface chemistry between Sb and TMDs, in particular MX<sub>2</sub> (M = Mo or W; X = S or Se), using X-ray photoelectron spectroscopy (XPS). Sb was deposited in ultra-high vacuum conditions (UHV) on bulk TMD surfaces, followed by annealing in UHV at 100°C, 200°C, and 300°C. The XPS measurements revealed an absence of chemical or interfacial reactions at room temperature, 100°C, and 200°C. However, upon annealing at 300°C, complete sublimation of the Sb layer was observed. These findings support the van der Waals nature of the interface, confirming that the interaction between Sb and the underlying TMDs remains non-reactive up to 200 °C. This thermal stability and inertness suggest that Sb could be a promising candidate for integration in 2D heterostructures and devices that require clean, weakly interacting interfaces.

[1] Y.-T. Lin et al. Nano Lett. (2024) 24, 8880–8886

[2] Z. Wang et al. Adv. Funct. Mater. (2023) 33, 230165

[3] T. Su et al. J. Phys. D: Appl. Phys. 56 (2023) 234001

[4] Wang et al. Adv. Funct. Mater. (2023) 33, 2301651

[5] Chou et al. IEEE International Electron Devices Meeting (IEDM), San Francisco, CA, USA (2021) 7.2.1-7.2.4.

9:00am **2D+AQS+EM+NS+QS+TF-FrM-4 Metal-to-Semiconductor Transition in Niobium Sulfoselenide Alloy and Niobium Sulfide Films by Compositional Control and Post Growth Sulfurization, Tinsae Alem, Abir Hasan, Kory Burns, Nikhil Shukla, Stephen McDonnell**, University of Virginia  
Transition metal dichalcogenides (TMD) have attracted increasing scientific interest due to their diverse properties including a tunable bandgap, optical anisotropy, low power consumption, and good elasticity. In this study, low-dimensional TMD films were grown with molecular beam epitaxy (MBE) to investigate the effects of varying chalcogen (sulfur and selenium) content in niobium sulfoselenide (NbS<sub>2</sub>Se<sub>2-x</sub>) alloys. Here, we focus on their electrical resistivity and electronic properties, including the transition from metallic to semiconducting behavior to have precise control over the material's electrical conductivity. Additionally, we analyzed the semiconductor-to-metal transition in NbS<sub>2</sub> films following post-growth sulfurization and the corresponding changes in resistivity. These MBE grown films were characterized using in-situ x-ray photoelectron spectroscopy (XPS) to analyze the chemical composition. Next, the electrical resistivity of films was calculated using their sheet resistance measured with a Jandel 4-point probe, and their thickness was estimated using x-ray reflectivity (XRR). We used transmission electron microscopy (TEM) to visualize these MBE-grown films at the atomic scale, enabling the correlation of atomic structure with electronic properties. Lastly, the temperature coefficient of resistance (TCR) measurements was performed to understand the resistivity of the films with temperature dependence and to determine their metallic and semiconducting behavior. Our results demonstrate that the transition from metal to semiconductor occurs with the addition of sulfur into the niobium selenide film. We also observed a trend of increasing resistivity as the sulfur content was increased in niobium selenide film. This work explores the potential of tuning the energy gap of TMD materials, making them ideal candidates for tunable nanoelectronics in various applications.

9:15am **2D+AQS+EM+NS+QS+TF-FrM-5 Evolution of the Electronic Gap of Directly Synthesized Versus Mechanically Transferred WS<sub>2</sub> Monolayer to Multilayer Films, Xu He, Antoine Kahn**, Princeton University

Transition metal dichalcogenides (TMDs) have emerged as promising electronics and optoelectronics materials for their strong light-matter interaction, large exciton binding energies, and bandgap tunability through the control of composition and the number of layers. Among TMDs, WS<sub>2</sub> stands out for its strong photoluminescence and spin-orbit coupling, making it ideal for exploring charge transfer and interfacial phenomena. However, discrepancies in reported energy levels (electronic gap, ionization energy, electron affinity) remain due to variations in growth and measurement methods, impeding device design.

In this study, we directly compare the band structure of WS<sub>2</sub> films from monolayer to multilayer (up to four layers) prepared by two commonly used methods: direct growth via metal-organic chemical vapor deposition (MOCVD) and mechanical exfoliation with layer-by-layer transfer. We utilize a suite of characterization techniques, including Raman spectroscopy, photoluminescence (PL), UV-vis absorption, and X-ray photoelectron spectroscopy (XPS), to probe vibrational modes and optical transitions. A combination of ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission spectroscopy (IPES) allows us to directly study the evolution of ionization energy and electron affinity, hence the electronic gap of the materials.

We find that the electronic gap (E<sub>g</sub>) of WS<sub>2</sub> consistently decreases with increasing layer number, reaching bulk-like values by the trilayer for mechanically transferred layers. The exfoliated monolayer is found to have an E<sub>g</sub> of 2.43 eV, which reduces to around 1.97 eV at the trilayer and stays at 1.98 eV for the tetralayer. This layer-dependent E<sub>g</sub> reduction is driven firstly by an upshift of the valence band maximum (VBM) at the 1L-2L transition and then by a downshift of the conduction band minimum (CBM) at the 2L-3L transition.

Comparing differently processed layers, we find the MOCVD-grown monolayer WS<sub>2</sub> to exhibit an electronic gap of 2.56 eV, larger than 2.43 eV for the mechanically transferred one. The slightly larger E<sub>g</sub> in MOCVD-grown monolayers also yields a higher exciton binding energy (~0.55 eV)

than in exfoliated monolayers (~0.43 eV). XPS analysis indicates that MOCVD samples contain more oxygen-related defect species, likely contributing to the subtle band gap differences and a small blue shift of their optical spectra relative to exfoliated layers.

Overall, this comparative study highlights the influence of the fabrication methods on the fundamental electronic structure of  $\text{WS}_2$ . These findings provide important guidelines for tailoring band alignments for  $\text{WS}_2$ -based heterostructures and optoelectronic devices.

**9:30am 2D+AQS+EM+NS+QS+TF-FrM-6 2D Phase Diagram of Iron Sulfides on Au(111): From Hexagonal to Square Atomic Arrangement and Beyond, Andrea Berti**, University of Trieste, Italy; **Marco Bianchi, Paolo Lacovig, Silvano Lizzit**, Elettra-Sincrotrone Trieste, Italy; **Philip Hofmann**, Aarhus University, Denmark; **Alessandro Baraldi**, University of Trieste, Italy

Despite extensive research on two-dimensional (2D) materials, almost all experimentally synthesized 2D systems derive from van der Waals crystals (vdW). While the use of vdW crystals has been remarkably successful, it inherently restricts the 2D materials landscape to compounds that are already layered in their bulk form. Less than 5% of known inorganic materials possess a layered structure suitable for exfoliation, and the vast majority of functional compounds—such as oxides, sulfides, and nitrides—do not belong to this category. In recent years, increasing efforts have focused on the realization of truly two-dimensional monolayers from non-vdW compounds, which could unlock novel properties in fields such as high-temperature magnetism, catalysis, and strongly correlated electron phenomena. Beyond the class of vdW materials, only a limited number of compounds have so far been theoretically predicted to be stable in the 2D limit. In this context, iron-sulfur compounds have recently emerged as promising candidates. Density functional theory predicts that both hexagonal  $\text{FeS}_2$  and tetragonal  $\text{FeS}$  phases can exist as stable monolayers, exhibiting strain-tunable magnetic properties. Although the Mermin-Wagner theorem precludes long-range magnetic order in ideal 2D isotropic systems, magnetic anisotropy can lift this constraint and allow stable ordering, enabling tunable magnetism at the atomic scale, which is essential for spintronics, as well as other emerging phenomena such as topological effects, multiferroicity, and proximity effects in heterostructures. However, compared to their bulk counterparts, Fe-S systems generally display a rich phase diagram, characterized by multiple stoichiometries and atomic arrangements. A similar complexity may also persist in the 2D limit, highlighting the need for a systematic experimental investigation into which 2D  $\text{FeS}_x$  phases can actually form. For this purpose, we systematically grow and characterize iron sulfide monolayers on Au(111) via in-situ co-deposition of Fe and S. Low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), and X-ray photoelectron spectroscopy (XPS) reveal two primary phases: one with a hexagonal atomic arrangement consistent with  $\text{FeS}_2$  (Fig. 1a), forming a moiré superstructure, and one with a square arrangement (Fig. 1b). By tuning sulfur exposure, we observe additional phases with varying stoichiometry and atomic arrangement, all belonging to the same  $5 \times 5$  superstructure family (Fig. 1c). These results confirm the existence of a complex 2D phase diagram for  $\text{FeS}_x$  monolayers, establishing them as a versatile and tunable platform for exploring 2D magnetism in non-vdW systems.

**9:45am 2D+AQS+EM+NS+QS+TF-FrM-7 The Electronic Band Structure and Conduction Band Formation of  $\text{HfSe}_3$ , Gauthami Viswanath**<sup>1</sup>, University of Nebraska-Lincoln, USA; **Alexey Lipatov**, South Dakota School of Mines and Technology; **Alexander Sinitskii**, University of Nebraska-Lincoln, USA; **Jose Avila**, Synchrotron SOLEIL and Université Paris-Saclay, France; **Takashi Komesu**, University of Nebraska-Lincoln, USA; **Maria C. Asensio**, Madrid Institute of Materials Science (ICMM), Spain; **Peter A. Dowben**, University of Nebraska-Lincoln, USA

**Abstract:** The anisotropic structure of Group 4 transition metal trichalcogenides (TMTCs) have gained significant interest due to their possible application in optoelectronics. In this work, the band structure of quasi one-dimensional  $\text{HfSe}_3$  was investigated with nano-spot angle resolved photoemission spectroscopy (nanoARPES).  $\text{HfSe}_3$  has a rectangular surface Brillouin zone where the effective hole mass along the chain direction is  $-0.27 m_e$  which is smaller compared to the effective hole mass along the direction perpendicular to the chains,  $-1.17 m_e$ . The effective hole mass extracted from the band structure along different high symmetry directions is compared with that of  $\text{TiS}_3$  and  $\text{ZrS}_3$  from prior studies.<sup>1</sup> X-ray absorption spectroscopy (XAS) has been used to characterize the unoccupied states of  $\text{HfSe}_3$  and will be compared to the XAS spectra of  $\text{HfS}_3$

<sup>2</sup> and  $\text{TiS}_3$  and  $\text{ZrS}_3$ .<sup>3</sup> The metal chalcogenide hybridization for Hf differs from the Ti and Zr trichalcogenides. This may be due to the increase in effective atomic number leading to strong spin-orbit interaction of Hf based TMTCs.

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**10:30am 2D+AQS+EM+NS+QS+TF-FrM-10 Applications of Two-dimensional Materials in Energy, Water, and Healthcare, David Estrada**, Boise State University

**INVITED**

The rapidly evolving field of 2-dimensional (2D) materials continues to open new frontiers in fundamental and applied research across water purification, healthcare, and energy applications. This talk will highlight our recent work in the synthesis of 2D and layered-materials-based inks, enabling energy innovations in microsupercapacitors, triboelectric nanogenerators, and electron devices [1-3]. In water applications, we introduce a flowing electrode capacitive deionization (FE-CDI) system utilizing  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene electrodes to efficiently remove and recover ammonia from synthetic wastewater and carbonates from simulated ocean water. This FE-CDI system demonstrates promising potential for managing nitrogen and carbon cycles while improving access to clean water [4]. In healthcare, the intersection of graphene and biology offers a powerful avenue for musculoskeletal tissue engineering, where graphene's exceptional physical properties contribute to fundamental biological insights [5-7]. Lastly, this talk will highlight recent insights into  $\text{WS}_2$  nucleation and film growth on sapphire using tungsten hexacarbonyl and hydrogen sulfide precursors in an AIXTRON 2D Close Coupled Showerhead MOCVD  $3 \times 2$  reactor, with in situ photoreflectometry monitoring. Together, these findings highlight the transformative role of 2D materials beyond graphene in addressing critical engineering challenges and advancing sustainable solutions across diverse fields.

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**11:00am 2D+AQS+EM+NS+QS+TF-FrM-12 Electronic Structure Modulation in 2D Metal-Graphene-Metal Electrocatalysts for  $\text{CO}_2$  Reduction and Hydrogen Evolution Reactions, Arturo Medina**, Ines Saih, Vikas Muralidharan, Georgia Institute of Technology; Jinwon Cho, NREL; Faisal Alamgir, Georgia Institute of Technology

Two-dimensional metal-graphene-metal (M/Gr/M) heterostructures provide a versatile platform for tuning electrocatalytic behavior through controlled interfacial strain and charge redistribution. In previous work, orbital-level descriptors were introduced to explain how pseudo-epitaxial strain alters the electronic structure of ultrathin metals, driving changes in

catalytic activity for the CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR). These concepts were grounded in density functional theory and validated experimentally by correlating spectroscopic strain signatures with shifts in catalytic onset potential.

Building on this framework, the present study expands the scope and range of electrocatalytic reactions studied in M/Gr/M systems. We integrate new measurements on the hydrogen evolution reaction (HER), exploring whether the same strain–electronic structure–reactivity relationships observed in CO<sub>2</sub>RR extend to HER kinetics. This includes analysis of onset potentials, overpotentials, and durability across a diverse set of M/Gr/M configurations. Various metals from the 3d to 5d series were investigated as candidate electrocatalysts, deposited as atomically thin layers on single-layer graphene. The graphene is supported by both metal and metal oxide substrates, enabling systematic modulation of ligand effects and interfacial bonding.

To probe strain and charge transfer, we employ a suite of synchrotron-based and lab-scale techniques including carbon K-edge near-edge X-ray absorption fine structure (NEXAFS), extended X-ray absorption fine structure (EXAFS), ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), and electron energy loss spectroscopy (EELS). We track strain-induced modifications in electronic structure through synchrotron-based spectroscopy, revealing systematic correlations between interfacial bonding, orbital structure, and catalytic performance. By comparing systems with and without graphene, we isolate the role of interfacial bonding in modulating both electronic structure and catalytic behavior.

This work experimentally explores theoretical predictions for HER in M/Gr/M systems and provides new insight into how strain-induced orbital modulation governs charge transfer and reactivity across multiple electrocatalytic reactions. Together, these results highlight M/Gr/M structures as a model system for disentangling the fundamental interactions between dimensionality, strain, and catalytic function.

**11:15am 2D+AQS+EM+NS+QS+TF-FrM-13 Large Area Nanostructuring of Van Der Waals Materials for Photon Harvesting in the Flat Optics Regime, Matteo Barelli<sup>1</sup>, Francesco Buatier de Mongeot, Simone Di Marco, University of Genoa, Italy; Rajesh Chennuboina, University of Genoa, India; Giorgio Zambito, Giulio Ferrando, University of Genoa, Italy; Matteo Gardella, CNR-IMM, Italy; Maria Caterina Giordano, University of Genoa, Italy**

2D-Transition Metal Dichalcogenides (2D-TMDs) are two-dimensional semiconductors featuring high optical absorption coefficient combined with good transport and mechanical properties. Although mechanically exfoliated TMDs flakes ensure the best optoelectronic properties, homogeneous large-area growth techniques are mandatory for real-world applications [1,2]. At the same time, in view of light conversion applications in the extreme thickness regime of 2D-TMDs, it is essential to develop effective photon harvesting flat optics strategies derived from nanophotonics.

Here we demonstrate that periodic modulation of few MoS<sub>2</sub> and WS<sub>2</sub> on large area nanostructured samples fabricated by laser interference lithography (either MoS<sub>2</sub> nanostripes arrays or conformal MoS<sub>2</sub> layers grown on top of nanogrooved silica templates). These nanopatterned layers can effectively steer light propagation via Rayleigh Anomalies in the flat optics regime, promoting strong in-plane electromagnetic confinement and broadband omnidirectional photon absorption enhancement, with strong impact in photoconversion. [3,4].

As a case study, we investigate the photocatalytic performance of periodically corrugated MoS<sub>2</sub> layers for photodissociation of Methylene Blue (MB), a widely used yet harmful textile dye. Under optimized angles coupling light to photonic anomalies, MB degradation is two times faster compared to planar MoS<sub>2</sub> films [5]. Additionally, periodic TMD nanostripes serve as directional scatterers, expanding possibilities for advanced light manipulation.

Another major challenge is the scalable fabrication of 2D van der Waals (vdW) heterostructures, often limited to micrometric flakes. Here, we demonstrate large-area (cm<sup>2</sup>-scale) nanoscale reshaping of vdW heterostructures. Specifically, we report a flat-optics platform using vertically stacked WS<sub>2</sub>-MoS<sub>2</sub> heterostructures endowed with type-II band alignment, forming periodic nanogratings [6]. These engineered large-area

vdW heterostructures enable scalable applications in nanophotonics, photoconversion [7], and energy storage.

We recognize funding by the NEST - Network 4 Energy Sustainable Transition - PNRR partnership.

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**11:30am 2D+AQS+EM+NS+QS+TF-FrM-14 Exploring the Temperature Coefficient of Frequency (TC<sub>f</sub>) in Graphene Trampoline Resonators, Yunong Wang, Nawara Tanzee Minim, S M Enamul Hoque Yousuf, Philip Feng, University of Florida**

In this work, we report the first experimental investigation of the temperature coefficient of resonance frequency (TC<sub>f</sub>) in graphene trampoline nanoelectromechanical system (NEMS) resonators. Trampoline resonators are widely used in photothermal sensing applications thanks to their superior thermal isolation, enabling high sensitivities. Leveraging the exceptional mechanical strength, thermal stability, and ultralow mass of two-dimensional (2D) materials, graphene trampoline resonators offer a compelling platform for ultrafast infrared (IR) detection. Characterizing the TC<sub>f</sub> is essential for designing sensors with stable performance across a wide temperature range, enabling high-resolution IR detection, and developing robust NEMS for advanced light sensing applications.

We use focused ion beam (FIB) to make trampoline structure on our graphene drumhead resonator. The resonance characteristics of the device are measured by using a laser interferometry system. An intensity-modulated 405 nm blue laser is employed to drive the device photothermally, and a 633 nm He-Ne laser is used to read out device resonance motions. The reflected light is detected by a photodetector and converted to an electrical signal, which is analyzed by a network analyzer to obtain the resonance response. To measure the resonance frequency at different temperatures, we regulate the temperature of the device with a metal ceramic heater. The temperature of the chip is measured by a platinum resistance temperature sensor.

We measure the resonance response of the device at different temperatures and extract the resonance frequency and quality (Q) factor by fitting the measured spectrum to the damped simple harmonic resonator model. The drumhead resonator with 20 μm diameter shows a resonance frequency  $f=3.44$  MHz and  $Q=528$ , while after FIB, the trampoline structure achieves a significantly higher  $f=13.03$  MHz and  $Q=5509$ . As temperature increases, the negative thermal expansion of graphene causes an upward shift in resonance frequency. We observe a TC<sub>f</sub> exceeding 30,100 ppm/°C from the drumhead structure, extracted from frequency shifts between 30 °C and 60 °C. After we FIB the drumhead structure into a trampoline, we found that the TC<sub>f</sub> reduced to 588 ppm/°C.

A lower TC<sub>f</sub> value from the stage heating-up method is desirable for stable operation across varying thermal conditions. Due to geometric isolation and reduced thermal coupling to the substrate, the trampoline is expected to exhibit a smaller TC<sub>f</sub> than its drumhead counterpart. This makes the trampoline resonator a strong candidate for IR sensing applications that require stable performance over a broad range of temperatures.



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