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,*** 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 AlOx-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**, ***Jerry Chow*** [1], IBM Quantum **INVITED**

9:15am **QS1-MoM-5 Stable Cnot-Gate on Inductively-Coupled Fluxoniums with Over 99.9% Fidelity – Part 1**, *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-$1/2$ 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 LC-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 – part 2**, ***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-$1/2$ 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 2×10^{-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 ~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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Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS2-MoM

Systems, Devices, and Manufacturing Technologies for Quantum Technology

Moderators: Sisira Kanhirathingal, Rigetti Computing, **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.

[1] **Quantum Keynote Lecture**

11:00am **QS2-MoM-12 Voltage Tunable MBE-grown Ge/SiGe Josephson Junctions for Gatemon Qubits**, ***Joshua Thompson***, *Jason Dong, Junior Langa,* Laboratory for Physical Sciences*; Brycelynn Bailey,* University of Arkansas*; Chomani Gaspe, Riis 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 cm^2/Vs and hole density less than $1x10^{12}$ cm^{-2}. These junctions use epitaxial aluminum to make transparent contact to the Ge-QW and a mesa structure that is 2.5-μm 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 gatemon qubits.

11:15am **QS2-MoM-13 An Even-Odd Superconducting Diode Effect in Topological Insulator Josephson Junctions**, ***Jonathan Zauberman***, Harvard University*; Joon Young Park,* Sungkyunkwan University (SKKU), Republic of Korea*; Thomas Werkmeister,* Harvard University*; Omri Lesser,* Cornell University*; Laurel Anderson,* University of Washington*; Yuval Ronen,* Weizmann Institute of Science, Israel*; Satya Kushwaha,* Johns Hopkins University*; Robert Cava,* Princeton University*; Yuval Oreg,* Weizmann Institute of Science, Israel*; Amir Yacoby, Philip Kim,* Harvard University

The superconducting diode effect (SDE), in which supercurrent is asymmetric in applied current bias, can be observed when time reversal and inversion symmetries are broken in a Josephson junction. Recently, changes in the sign of the SDE have been correlated with possible topological phase transitions in certain regimes of linear Josephson junctions. Here we report an even-odd SDE in Corbino-geometry Josephson junctions, where even/odd flux parity states show a SDE alternating in sign. These junctions are fabricated on a single surface of a bulk-insulating three-dimensional topological insulator and can be used for probing signatures of Majorana states that are theoretically present within the junctions under a magnetic field. We fabricate high-quality niobium Josephson junctions on tellurium-capped Sn-doped $Bi_{1.1}Sb_{0.9}Te_2S$ (Sn-BSTS) single crystals, with junctions showing high transparency. Additionally, different Corbino-style geometries enable Josephson interferometry within a single junction, allowing us to explore the skewed current-phase relation. Our analysis attributes the flux-parity controlled SDE to a topological phase, with opposite diode polarity directly reflecting the sign change of the periodic boundary conditions for an even/odd number of Josephson vortices in the junction.

11:30am **QS2-MoM-14 Post-processing of Josephson Junctions for Precision Tuning of Qubit Frequencies** , ***David P. Pappas***, 775 Heinz Ave*; 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 Laboatory*; 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.

12:00pm **QS2-MoM-16 Probing the Nonlinearities of Nb-Doped a-Si Josephson Junctions with Microwave Intermodulation Spectroscopy and Large-Signal Network Analysis**, ***Elyse McEntee Wei***, Colorado School of Mines; NIST*; Dylan Williams, Christian Long,* NIST-Boulder*; Serena Eley,* University of Washington

Niobium-doped amorphous silicon Josephson junctions are used in a variety of applications, such as the Josephson Programmable Voltage Standard and the Josephson Arbitrary Waveform Synthesizer. The operating parameters required of each application dictate the amount of niobium doping in the amorphous silicon barriers. By increasing the niobium doping concentration, the junction behavior can be tuned from superconductor-insulator-superconductor type junctions to superconductor-normal metal-superconductor or superconductor-weak superconductor-superconductor type junctions. Preliminary studies of these junctions suggest that the dependence of the supercurrent in the barrier on the phase difference of the superconducting order parameters (known as the current-phase relation) begins to deviate from a simple sinusoid with increasing concentrations of niobium. Although the skewing of the current-phase relation is suspected to influence the harmonic output of the device and significantly affect the device behavior, this correlation between the varying degrees of skewing and harmonic output is largely unexplored. Here we investigate two techniques to probe the nonlinear response of niobium-doped amorphous silicon Josephson junction arrays embedded in on-wafer niobium superconducting transmission lines. First, we perform on-wafer intermodulation spectroscopy by stimulating the Josephson junction arrays with two microwave tones and measuring the resulting intermodulation products to extract the current-phase relation. We then perform large-signal network analysis (involving a two-tier microwave calibration that includes absolute power and cross-frequency phase calibrations) to capture the harmonic spectral response of the junctions at the cryogenic device reference plane. Upon the successful combination and implementation of these two techniques, we will have developed a method to measure the current-phase relation and the resulting harmonic spectrum of a device in a single setup. By analyzing the current-phase relation's dependence on the niobium doping concentration and its effect on the harmonic output of a device, we can improve our device models to accurately predict a device's behavior in an application, leading to improved device design and performance.

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 Growth and Characterization of Thin-Film A15 Nb-Al Intermetallics for Superconducting Quantum Electronics**, ***Joseph Falvo***, 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 Nb3Al, 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 Tc greater than 16 Kelvin and zero-temperature critical fields greater than 30 T. Additionally, we report single-photon microwave quality factors of 1.9x105 and estimates for kinetic inductance similar to NbN at comparable thickness.

1:45pm **QS1-MoA-2 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 GΩ*um^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 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 ≈ 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.

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 $Si_{0.2}Ge_{0.8}$ virtual substrates. The $Si_{0.2}Ge_{0.8}$ 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 cm^2/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 µm 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 Spatially and Spectrally controlled MBE Grown InAs/GaAs Quantum Dots for Device Platforms**, ***Nazifa Tasnim Arony***, University of Delaware; *Lauren N. McCabe,* University of Delaware (Now at Yale University); *Joshya Rajagopal, Lan Mai, Lottie Murray, Prashant Ramesh, Matthew Doty, Joshua Zide,* University of Delaware

InAs quantum dots (QDs) grown epitaxially on GaAs substrates have emerged as promising candidates for single-photon emitters, particularly due to their compatibility with established semiconductor manufacturing techniques. This compatibility paves the way for scalable quantum devices in fields like quantum sensing, computing, and information processing. However, for the production of fully functional epitaxial quantum devices on a large scale, uniformity in spatial, spectral, and structural properties, along with scalability, is essential. Recent work from our group has introduced a method for site-controlled QD growth, where InAs/GaAs QDs are grown on nano-fabricated substrates featuring site-templated arrays of nano-pits [1]. Despite these developments, fabrication processes often introduce impurities that can adversely affect their optical performance, and hence, maintaining high-quality optical emission from these site-controlled QDs is still a major challenge. In response to this issue, this study investigates the use of quantum dot columns (QDCs) as a buffer layer above the initial site-templated QD arrays. This approach effectively "buries" defects beneath the QDCs, thereby enhancing the optical quality of the top QDs of interest. Additionally, we present initial photoluminescence (PL) data showcasing the spectral control over InAs/GaAs QDs achieved through the 'cap and flush' technique, which enables the tuning of their emission properties.

[1] J. Vac. Sci. Technol. B 38, 022803 (2020)

2:30pm **QS1-MoA-5 Epitaxy of Superconducting Germanium Thin Films for Integrated Quantum Electronics**, ***Patrick Strohbeen***, New York University; *Julian Steele, Ardeshir 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.

2:45pm **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 Univeristy

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 $Ca(OH)_2$ targets. X-ray fluorescence reveals that metallic calcium targets contain substantial chlorine impurities, which adversely affects CaO film growth via sputtering. We demonstrate $Ca(OH)_2$ 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 $Ca(OH)_2$ target during sputter deposition. Deposition growth rates achieved from the $Ca(OH)_2$ 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 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**, ***Arany 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). TLS's reduce coherence times and increase temporal fluctuations, making qubits harder to operate in a system. One of the major sources of such TLS's 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 Tc = 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.

This material is based upon work supported under Air Force Contract No. FA8702-15-D-0001. Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the U.S. governement or the U.S. Air Force.

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.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Superconducting Quantum Materials and Systems Center (SQMS) under contract number DE-AC02-07CH11359.

5:00pm **QS2-MoA-15 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 10^21cm^-3, that yield superconductivity with a critical temperature of Tc = 3.5K. 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.

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

8:00am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-1 Optical Integration for Trapped-Ion Systems*, Daniel Stick,*** Sandia National Laboratories **INVITED**

First demonstrated in 2006, surface ion traps provide a platform for storing 2D arrays of ions and have been widely adopted across the trapped-ion quantum computing community. To take advantage of the scalability enabled by these devices, on-chip waveguides have been developed over the last decade to replace traditional bulk-optics that can only illuminate a single line of ions. Here I will describe integrated photonics experiments that bring together multiple elements to control larger arrays of ions, as well as new approaches to addressing the I/O challenge of bringing the many optical signals across the ultra-high vacuum boundary. These advances are necessary for supporting the large number of ions needed for trapped-ion quantum computing, as well as for making deployable optical clocks.

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 he 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_4 or As_2, and with a wide range of arsenic beam equivalent pressures, from $5x10^{-7}$ to $1x10^{-5}$ 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.

1. Krishtopenko and Teppe. *Science Advances* **4**, eaap7529 (2018)
2. Avogadri et al. *Physical Review Research* **4**, L042042 (2022)
3. Du et al. *Physical Review Letters* **119**, 056803 (2017)

8:45am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-4 Benchmarking different NbTiN sputtering methods for 300 mm CMOS-compatible superconducting digital circuits*, Adham Elshaer, 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 Tc, 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 Tc 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_3As_2 and the formation and behavior of domain boundaries in the Weyl TSM TaAs.

This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Research was performed under the Disorder in Topological Semimetals project funded by the U.S. Department of Energy Office of Science, Basic Energy Sciences, Physical Behavior of Materials program. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

9:30am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-7 Photon Down-Conversion of Yb-Doped CsPb(Cl1-xBrx)3 to Low-bandgap Metal Halide Perovskites***, **Yutong Ren**,* 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.[1,2] 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 $CsPb(Cl_{1-x}Br_x)_3$, 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.

Our investigation focuses on elucidating the structural and electronic properties of the interfaces between Yb-doped $CsPb(Cl_{1-x}Br_x)_3$ 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 $CsPb(Cl_{1-x}Br_x)_3$ 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.

1. Wegh, R. T. et al. Quantum cutting through downconversion in rare-earth compounds. *J. Lumin.* **87–89**, 1017–1019 (2000).

2. Kroupa, D. M. et al. Quantum-cutting ytterbium-doped $CsPb(Cl_{1-x}Br_x)_3$ perovskite thin films with photoluminescence quantum yields over 190%. *ACS Energy Lett.* **3**, 2390–2395 (2018).

9:45am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-8 Implementation of a Truly 2D Model to Describe the Weak Antilocalization Behavior of Topological Insulators***, **Ryan Van Haren**, Aubrey Hanbicki, Adam Friedman,* Laboratory for Physical Sciences

Topological insulators continue to garner interest for potential and functionally-prototyped applications in next-gen electronic, spintronic, and quantum devices. In many of these applications, the topological surface states play a critical role. Transport through the surface states is often quantified by fitting to quantum corrections to the conductance that appear at low temperature. The model commonly used for these fittings is the Hikami-Larkin-Nagaoka (HLN) model, a quasi-2D model that does not account for the Dirac nature of the topological surface state. In the years following the discovery of topological insulators, theoretical work was performed that calculated the quantum corrections while taking into account the unique properties of the topologically protected surface states[1]. This Dirac fermion model provides powerful insight into the surface state transport by quantifying the Fermi velocity and the phase coherence length, among other parameters, but adoption of this model has been slow due to it being more complicated to utilize than the HLN model. In this work, I will present my method for implementing the Dirac fermion model in practice on weak antilocalization data from topological insulator thin films of $Bi_{0.85}Sb_{0.15}$ and previously published topological insulator thin films[2]. I will contrast the Dirac fermion model fits with the HLN model fits and show how the derived Fermi velocity agrees well with values derived from ARPES measurements reported in literature. I will make the argument that, while the HLN model still has its uses, analysis of weak antilocalization behavior in topological insulators is incomplete without utilization of the Dirac fermion model.

(1) Adroguer, P.; Liu, W. E.; Culcer, D.; Hankiewicz, E. M. Conductivity Corrections for Topological Insulators with Spin-Orbit Impurities: Hikami-Larkin-Nagaoka Formula Revisited. *Phys. Rev. B* **2015**, *92* (24), 241402. https://doi.org/10.1103/PhysRevB.92.241402.

(2) Van Haren, R.; Lederman, D. Suppressed Weak Antilocalization in Topological Insulator--Antiferromagnetic Insulator $(BiSb)_2Te_3$-MnF_2 Thin Film Bilayers. *Phys. Rev. B* **2024**, *110* (20), 205409. https://doi.org/10.1103/PhysRevB.110.205409.

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 CdSexTe1-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 CdSexTe1-x has emerged as a key candidate for enhancing the short-circuit current (Jsc) by lowering the bandgap below 1.45 eV, which could help push short-circuit-current (Jsc) closer to its theoretical limits.

In this study, we fabricated $CdSe_xTe_{1-x}$/CdTe devices with vapor transport technology (VTD) and characterized the structural chemistry and electronic properties of $CdSe_xTe_{1-x}$/CdTe devices from the carrier collection dynamics perspective. The device structure is CdSeTe/CdTe absorbers on TEC-10 glass coated with fluorine-doped tin oxide (SnO_2: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 $ClCl_2$ ambient at 480 C for grain recrystallization and grain boundary passivation. Selenium (Se) diffuses deeper into the CdTe film to form 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 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^2. The Se concentration is approximately 5-7 %, incorporated into the front interface of $CdSe_xTe_{1-x}$/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 $CdSe_xTe_{1-x}$/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^2, whereas the red light charge collection is 4.37 mA/cm^2. The most charge collection occurs at in-between wavelengths as 18.71 mA/cm^2.

11:15am **EM2+AP+QS+TF-TuM-14 Analysis of $KNbo_3$ Crystal Structure Fabricated on $LiNbO_3$ and $LiTaO_3$ 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 $KNbO_3$ are in focus for new type of sensors and electronic materials due to its high piezoelectric properties, high curie temperature around 450℃ 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 ($LiNbO_3$) and lithium tantalate ($LiTaO_3$) 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 $KNbO_3$film were synthesis on $LiNbO_3$,$LiTaO_3$ single crystals substrate by hydrothermal method aiming for possibility of electro-optical switching devices, energy conversion and other sensing devices.

$KNbO_3$ (100) and (111) structure epitaxially grown on $LiNbO_3$ and $LiTaO_3$ 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 $KNbO_3$ film synthesis on $LiNbO_3$ and $LiTaO_3$ which is important for piezo electric properties [5].

[1] T. Stevenson, D. G. Martin, P.I. Cowin, A. Blumfield, A. J. Bell, T. P. Domyn, P. M. Wearver, Piezoelectric materials for high temperatures transducers and actuators, J. Matter. Scpi. Mater Electron 26, 9256-9267, 2015.

[2] Ryo Kudo, Peter Bornnann, Tobias Hemsel and Takeshi Morita, Thick KNbO3 film deposited by ultrasonic-assisted hydrothermal method, acoust. Sci. & Tech. 36, 3262-264, 2015.

[3] T. Stevenson, D. G. Martin, P.I. Cowin, A. Blumfield, A. J. Bell, T. P. Domyn, P. M. Wearver, Piezoelectric materials for high temperatures transducers and actuators, J. Matter. Scpi. Mater Electron 26, 9256-9267, 2015.

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[5] Xiaoyan Liu, Kazuya Terabe and Kenji Kitamura, Stability of engineered domains in ferroelectric LiNbO3, LiTaO3, crystals, Phys. Scr. T129, 103-107, 2007.

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-κ 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

Moderators: Andre Schleife, University of Illinois at Urbana-Champaign, **Sisira Kanhirathingal**, Rigetti Computing

8:00am **QS1-TuM-1 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 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 Externship 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.

8:15am **QS1-TuM-2 Quashing Logical Errors with Multimode Quantum Error Correction**, *Nick Frattini, Dany Lachance-Quirion,* ***Matthew Hamer***, *Marc-Antoine Lemonde,* Nord Quantique, Canada

Quantum error correction (QEC) is essential for fault-tolerant quantum computing, ensuring that logical informationremains protected from physical noise during the execution of quantum algorithms. Traditional QEC strategies achieve this by redundantly encoding logical qubits across many physical qubits, incurring significant hardware overhead. At Nord Quantique, we leverage the large Hilbert space of quantum oscillators to perform QEC within a single physical system, offering a potentially more hardware-efficient path to fault-tolerant quantum computing.

Among such bosonic codes, grid codes are particularly promising, as they encode discrete-variable logical information in translationally invariant lattices in phase space. Recent experimental demonstrations in superconducting circuits have validated this approach with single-mode grid codes, enabling QEC that helps more than it hurts. A key challenge in these demonstrations were the silent logical errors induced by auxiliary control systems (e.g., transmons). One promising avenue to circumvent this for FTQC are multi-mode grid codes, where auxiliary errors may move the state outside of the logical space rather than inducing silent logical errors.

In this talk, we will present our experimental resultsalong two axes toward FTQC: gates for single-mode grid qubits, and QEC for two-mode grid qubits. For the two-mode so-called tesseract code, we will demonstrate its

enhanced features by leveraging mid-circuit measurement outcomes to suppress logical decay in a hardware-efficient architecture.These results validate Nord Quantique's vision of multimode grid codes as a promising pathway toward FTQC.

8:30am **QS1-TuM-3 Quantum Information Processing Stack: From Bottom to Top and Back**, ***Sophia Economou,*** 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.

9:00am **QS1-TuM-5 Quantum Simulation of Condensed Matter Using Trotterized Entanglement Renormalization**, ***Thomas Barthel,*** Duke University

Strongly-correlated quantum matter can be simulated with tensor network states. A very interesting approach, motivated by real-space renormalization group, is the multi-scale entanglement renormalization ansatz (MERA). While MERA has various advantages over alternative tensor network methods, it has relatively high classical computation costs, which limits the attainable approximation accuracy [1]. To avoid the classically expensive contractions of high-order tensors, we have developed a variational quantum eigensolver (VQE) based on MERA and tensor Trotterization [2]. Due to its causal structure and noise-resilience, the MERA VQE can be implemented on noisy intermediate-scale (NISQ) devices and still describe large physical systems. The number of required qubits is system-size independent and only grows logarithmically when using quantum amplitude estimation to speed up gradient evaluations. Translation invariance can be used to make computation costs square-logarithmic in the system size and describe the thermodynamic limit. Results of benchmark simulations for various critical spin models and algorithmic phase diagrams substantiate a quantum advantage [3] and we have proven the absence of barren plateaus [4-6]. I will report on first experimental tests on ion-trap devices, which clearly demonstrate a continuous quantum phase transition. Using a new holographic tomography scheme, we were also able to resolve for the first time the transition from area-law to log-area law scaling of subsystem entanglement entropies when approaching criticality [7].

[1] "Scaling of contraction costs for entanglement renormalization algorithms including tensor Trotterization and variational Monte Carlo", arXiv:2407.21006, PRB 111, 045104 (2025)
[2] "A quantum-classical eigensolver using multiscale entanglement renormalization", arXiv:2108.13401, PRR 5, 033141 (2023)
[3] "Convergence and quantum advantage of Trotterized MERA for strongly-correlated systems", arXiv:2303.08910, Quantum 9, 1631 (2025)
[4] "Absence of barren plateaus and scaling of gradients in the energy optimization of isometric tensor network states", arXiv:2304.00161, Commun. Math. Phys. 406, 86 (2025)
[5] "Isometric tensor network optimization for extensive Hamiltonians is free of barren plateaus", arXiv:2304.14320, PRA 109, L050402 (2024)
[6] "Equivalence of cost concentration and gradient vanishing for quantum circuits: An elementary proof in the Riemannian formulation", arXiv:2402.07883, Quantum Sci. Technol. 9, 045039 (2024)
[7] "Probing entanglement scaling across a quantum phase transition on a quantum computer", arXiv:2412.18602

9:15am **QS1-TuM-6 Reducing the Resources Required by ADAPT-VQE Using Coupled Exchange Operators and Improved Subroutines**, ***Mafalda Francisco Ramôa da Costa Alves,*** Virginia Tech, Portugal; *Sophia Economou, Edwin Barnes, Nicholas Mayhall, Panagiotis Anastasiou,* Virginia Tech; *Luis Santos,* INESC TEC, Portugal

Adaptive variational quantum algorithms arguably offer the best prospects for quantum advantage in the NISQ era. Since the inception of the first such algorithm, ADAPT-VQE, many improvements have appeared in the literature. We propose two modifications to the algorithm: (i) a Hessian recycling protocol, where the approximate second derivatives of the cost function obtained by quasi-Newton optimizers flow from one iteration to the next, and (ii) a novel operator pool, the Coupled Exchange Operator (CEO) pool, where the elements are linear combinations of qubit excitations. We show that unitaries generated by CEOs can be implemented with low two-qubit gate counts - in particular, they can be implemented with as many or fewer CNOTs as those generated by only one of the constituent qubit excitations.We combine these two improvements with others previously proposed in the literature to create the most cost- and hardware-efficient version of ADAPT-VQE to date. We use the resulting algorithm on a range of molecular systems, and assess the cost of executing it on hardware. We show a dramatic reduction of these quantum resources compared to prior versions of the algorithm and find that our state-of-the-art CEO-ADAPT-VQE outperforms UCCSD, the most widely regarded static VQE ansatz, in all relevant metrics.We further compare the algorithm to state-of-the-art static ansatze and observe that all those with a comparable CNOT count to ADAPT-VQE require a measurement overhead of the order of 10^5 for small (12 qubit) molecules. This goes against the common belief that the adaptive ansatz construction incurs a measurement overhead - thanks to ADAPT-VQE-specific cost optimizations and the favorable cost landscape the algorithm naturally generates, the measurement costs are actually decreased.

9:30am **QS1-TuM-7 Floquet-ADAPT-VQE: A Quantum Algorithm to Simulate Non-Equilibrium Physics in Periodically Driven Systems**, ***Abhishek Kumar,*** *Karunya Shirali, 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 is 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 Characterization and Comparison of Optoelectronic Properties of High-Internal Quality Factor, Superconducting TiN Devices Deposited Using Molecular Beam Epitaxy and Magnetron Sputtering**, ***Elizabeth Pogue***, *Adrian Podpirka, Andrew Bennett-Jackson, James Shackford, Jeff Corgan,* Johns Hopkins Applied Physics Lab*; Thomas Whorisky,* Johns Hopkins University*; Joseph Prestigiacomo,* Naval Research Laboratory*; Austin Ferrenti,* Johns Hopkins University*; D. Scott Katzer, Virginia Wheeler,* Naval Research Laboratory*; Kyle McElroy,* Johns Hopkins Applied Physics Lab

Superconducting nitrides are of interest for a wide variety of quantum computing, quantum sensing, and quantum circuit applications. In contrast to conventional elemental superconductors like Nb and Al, superconducting nitrides are amenable to epitaxy with insulating nitrides, SiC, sapphire, and silicon. Superconducting nitrides also offer substantial tunability in properties like the superconducting gap and degree of crystallinity. This tunability feature also introduces challenges as the deposition conditions of these nitrides impact the performance of and decoherence mechanisms in play for these end-use applications. Here, we compare changes in kinetic inductance and optical properties of TiN resonators made using MBE and sputtered TiN films. We show that devices made from sputtered TiN films exhibit kinetic inductance two orders of magnitude higher than the devices made from MBE-grown TiN films, despite relatively similar IR properties. The MBE-grown TiN resonators exhibit kinetic inductances < 1 pH/sq with RRR >5.5. The analysis approaches needed for extracting kinetic inductance from such well-ordered films, which require more care than films with more disorder, are described. We show limitations of conventional methods used to extract resonator quality factor; when the external quality factor is lower than the internal quality factor, measurement line non-linearities have a pronounced impact on characterization.

11:45am **QS2-TuM-16 Invited Paper**, ***Irfan Siddiqi***, Lawrence Berkeley National Laboratory **INVITED**

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 Exploration and Synthesis of Uranium and Uranium Ditelluride Thin Films**, ***Colin Myers****, Deepak Kumar,* University of Maryland, College Park*; Kasra Sardashti,* Laboratory for Physical Sciences*; Johnpierre Paglione,* University of Maryland, College Park

Uranium Ditelluride (UTe2) has recently emerged as one of the most interesting superconducting materials to date. Possessing a superconducting transition temperature Tc ≈ 1.8 K, this heavy fermion exhibits unconventional spin-triplet superconductivity, suggested to be caused by spin fluctuations. With highly anisotropic critical fields up to 35 T and evidence of topological superconductivity, UTe2 garners significant interest as a candidate not only to study exotic superconductivity but also for integration into superconducting devices and quantum computation. The majority of research on UTe2 has been done on bulk crystals with shockingly little in the way of thin film studies. This is in part due to the challenging nature of incorporating tellurium, a low-vapor-pressure material, with heavy uranium atoms on a heated substrate. Epitaxial growth of UTe2 films becomes increasingly difficult when trying to fine-tune substrate temperature, lattice mismatch, and annealing times. Here, we present an approach to UTe2 film growth via pulsed laser deposition with consideration of epitaxial uranium and an overview of progress on UTe2 thin film growth.

2:45pm **QS1-TuA-3 Enabling Quantum Information Science with DNA-Templated Quantum Materials**, *Xin Luo, 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 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.

4:00pm **QS1-TuA-8 Strain-Engineered Tin-Vacancy Qubits in Diamond: In-situ Synchrotron based Structural and Optical Probes at operational Temperatures**, ***Philip Ryan****,* Argonne National Laboratory, USA

Next-generation quantum technologies demand precise control over the structural and electronic environment of solid-state qubits. Group IV color centers in diamond, particularly tin-vacancy (SnV) defects, have emerged as promising spin-photon interfaces due to their high optical coherence and symmetry-protected electronic states. However, practical deployment of these qubits is limited by low-temperature operational requirements driven by phonon-mediated decoherence.

This presentation will highlight a new synchrotron-enabled experimental platform under development to directly correlate local atomic structure and strain-induced quantum optical response in SnV qubits in diamond. Using micron-resolved high-resolution X-ray diffraction and diffuse scattering at the Advanced Photon Source, combined with integrated cryogenic photoluminescence spectro-microscopy, we are enabling in-situ studies of

qubit behavior under extreme uniaxial tensile strain below 2 Kelvin temperatures.

The platform is based on a Joule-Thomson driven cryostat engineered for sub-2K operation, with nanometer positional control and wide-angle X-ray access. Strain engineering leverages enhanced spin-orbit coupling to suppress decoherence pathways, with the ultimate aim of achieving coherent qubit operation at liquid nitrogen temperatures.

This capability will resolve how long-range strain fields, local defect environments, and lattice disorder influence spin coherence and phonon scattering—key mechanisms governing both quantum state lifetimes and optoelectronic coupling. Our approach represents a new paradigm in synchrotron-enabled quantum materials research and paves the way for scalable, strain-tunable quantum devices.

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

4:15pm **QS2-TuA-9 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. NitrogenVacancy (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 TinVacancy (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 Focussed 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.

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 (≥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 (Er^{3+}), which has an optical transition in the telecom range at ∼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 Er^{3+} ions in these nanostructures via advanced nanofabrication and implantation engineering and 2) an enhanced effective excitation cross-section (~6×10^{-18} cm^2). By leveraging these innovations, we have successfully isolated and characterized single and few-erbium ions in SiC NWs and HNPs at temperatures of ≥77 K—otherwise unattainable in bulk materials. Furthermore, through nanofabrication engineering and the minimization of implantation-induced defects, we have demonstrated single-photon Er^{3+} emission with a narrow optical linewidth of 90 MHz and single-Er^{3+}-ion qubit control, performed by Rabi oscillations in the optical domain and at temperatures of ≥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 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 Investigating Processing Spaces of Epitaxially Grown Nitride Materials with Quantum and Conventional Supervised Learning**, ***Andrew Messecar***, 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.

*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).

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 ultimate1000X 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 that 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 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, CeO2), 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

Moderators: Peter Sutter, University of Nebraska, **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 constraint 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_2 layer CVD and TMD oxidation phenomena, and howdirect 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,*** *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_2Se_3 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_2Se_3 on Al2O3 (0001) and Si (111) substrates using an atomic layer deposition SiO2 mask. Etching of the SiO2 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_2Se_3 film. First, we will discuss the effects of different substrate temperatures on the selective growth of the Bi_2Se_3 thin films. Second, we will discuss the geometric influence of variously 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,*** *Sumner B. Harris,* Oak Ridge National Laboratory, USA*; Austin Houston,* University of Tennessee Knoxville*; Ivan Vlassiouk,* Oak Ridge National Laboratory, USA*; Alexander Puretzky,* Oak Ridge Natinal 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,*** 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 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 μm (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[1] and SnS van der Waals ferroelectrics.

Finally, we demonstrate the integration of the ultrathin ferroelectric SnSe and SnS into lateral heterostructures.[2] 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,[1] making it a promising candidate for nanoelectronics such as field effect transistors (FETs).[2] SnSe in the orthorhombic *Pnma* structure exhibits significant electrical anisotropy where thecarrier mobility is 45% higher along the [010] direction than the [001] direction in plane,[3] 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,[4] 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 uncleaved 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.[5] 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.

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5:30pm **2D+EM+NS+QS+SS+TF-WeA-14 Synthesis of Millimeter-Scale Single-Crystal α-MoO_3 Nanosheets on Sapphire***, **Ryan Spangler**,* Pennsylvania State University*; Thiago Arnaud, Joshua Caldwell,* Vanderbilt University*; Jon-Paul Maria,* Pennsylvania State University

α-MoO_3 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, α-MoO_3 exhibits extreme anisotropy of the dielectric function, enabling in-plane and out-of-plane elliptic or even hyperbolic behavior at various wavelengths. Therefore, α-MoO_3 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 α-MoO_3. In this work, we describe a process for the growth of ultra-large, thin, and atomically smooth single crystals of α-MoO_3 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_3 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 α-MoO_3 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 α-MoO_3 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_2 Grown by CVD**, ***Elycia Wright***, *Kedar Johnson, Amari Gayle, Robin Rouseau, M.K. Indika Senevirathna, Michael D. Williams,* Clark Atlanta University

Rhenium disulfide (ReS_2) 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_2 holds remarkable properties, including anisotropic electronic, optical, and mechanical characteristics. Unlike other TMDs such as MoS_2, $MoSe_2$, WS_2, and WSe_2, ReS_2 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_2 particularly promising for applications in highly responsive photodetectors. To maximize the potential of ReS_2 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_2 can lead to variations in growth rates in different directions, resulting in multidomain structures that complicate the production of single-crystal ReS_2 on a large scale.

In this study, we will synthesize ReS_2 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_2.

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^2/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

Moderators: Shengxi Huang, Rice University, **Daniel Yimam**, Oak Ridge Natinal 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 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 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.

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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 Puretzky,* 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 Geohegan,* 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 MoS_2 and highly defective 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 MoS2 / WS2 @ 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 MoS_2 and 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 MoS_2 and WS_2 deposited on 1L h-BN-capped gold we observed in TERS spectra, completely unexpectedly, appearance of Raman bands at about 796 cm^{-1} and 76 cm^{-1} which are not normally observed in regular Raman spectra of h-BN or WS_2/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 MoS_2 and WS_2 deposited on the monolayer h-BN capped gold, moreover, the 796 cm^{-1} band often was the strongest band observed in TERS spectra, even stronger than A' mode from WS_2 or 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 WSe_2,$MoSe_2$, and 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 $MoSe_2$ and WSe_2 @ 1L h-BN@Au, while WS_2 monolayers deposited on the same substrate as WSe_2, showed expected response. More importantly, the excitation laser wavelength dependence in our case was completely different from what was reported earlier: in 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 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 $MoTe_2$**, ***Onyedikachi Alanwoko,*** *Nirosha 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 $MoTe_{2-x}$ 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 $MoTe_2$ 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 $MoTe_2$ with dissimilar transition metals to create new doped or alloyed 2D materials with potentially desirable properties.

9:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-8 Quantum Confining Excitons with Electrostatic Moiré Superlattice***, Liuxin Gu, Lifu Zhang, Sam Felsenfeld,* University of Maryland, College Park*; Rundong Ma,* University of Maryland College Park*; Suji Park, Houk Jang,* Brookhaven National Laboratory*; Takashi Taniguchi, Kenji Watanabe,* National Institute for Materials Science, Japan*; You Zhou,* University of Maryland, College Park

Quantum confining excitons has been a persistent challenge in the pursuit of strong exciton interactions and quantum light generation. Unlike electrons, which can be readily controlled via electric fields, imposing strong nanoscale potentials on excitons to enable quantum confinement has proven challenging. In this study, we utilize piezoelectric force microscopy to image the domain structures of twisted hexagonal boron nitride (hBN), revealing evidence of strong in-plane electric fields at the domain boundaries. By placing a monolayer $MoSe_2$ only one to two nanometers away from the twisted hBN interface, we observe energy splitting of neutral excitons and Fermi polarons by several millielectronvolts at the moiré domain boundaries. By directly correlating local structural and optical properties, we attribute such observations to excitons confined in a nanoscale one-dimensional electrostatic potential created by the strong in-plane electric fields at the moirédomain boundaries. Intriguingly, this 1D quantum confinement results in pronounced polarization anisotropy in the excitons' reflection and emission, persistent to temperatures as high as ~80 Kelvins. These findings open new avenues for exploring and controlling strongly interacting excitons for classical and quantum optoelectronics.

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.[1] 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,[2] which for the first time allowed the identification of chirality effects in the photonic properties of a single nanostructure.[3] 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.

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11:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16 Electrical Manipulation of Valley Polarized Charged Excitons in 2d Transition Metal Dichalcogenides***, Kuan Eng Johnson Goh,* Agency for Science Technology and Research (A*STAR), 2 Fusionopolis Way, Innovis #08-03, Singapore 138634, Singapore

The control of excitons in 2-dimensional (2D) Transition Metal Dichalcogenide (TMD) semiconductors is a key enabler for their use in optoelectronic, valleytronic and quantum applications. Reproducible electrical control of excitons remains elusive as excitons are intrinsically charge neutral quasiparticles. Here, we demonstrate that charge defects present in 2D TMDs like single-layer H-phase WS_2 [1,2], could be advantageous for electrical control through the coherent coupling of the exciton or biexciton with intrinsic charges in the single-layer WS_2, thus enabling a simple and robust method for electrical manipulation of the degree of valley polarization from <10% to >60% [3]. Such robust electrical tunability of the spectral resonance of the charged states indicates resonant control of valley polarization by exploiting the intricate interplay between the charged and neutral exciton/biexciton states, representing a key advance towards using the valley degree of freedom as an alternate information carrier.[4].

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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 revealshow 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 showsdifferent 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 relevant2D materials for scalability.

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 FeTe0.55Se0.45. 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 $MoTe_2$**, ***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 $MoTe_2$-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_2-Bi_2Se_3**, *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 Bi2-Bi2Se3 using scanning tunneling microscopy (STM) and conductive atomic force microscopy (C-AFM). Bi2-Bi2Se3 is an intrinsic superlattice material s comprised of a Bi2Se3 quintuple layer (QL) slab and a 2D Bismuthine (Bi2) 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 Bi2Se3 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 Bi2-Bi2Se3. 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_2**, ***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_2, 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_2 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_2 films on a gate tunable graphene field effective transistor supported by hBN. Gate-dependent STS reveals a substantial energy gap in 1T'-WTe_2 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 (CrI3) and progressive steps towards realizing moiré magnetism. Noting that bilayer CrI3 is a layered antiferromagnet and that any homogeneous stacking of two bilayers necessarily produces zero magnetization, we have revealed, in twisted double bilayer CrI3, 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.

4:15pm **2D+AQS+MI+NS+QS+TF-ThA-9 High-Efficiency Optoelectronic Training of Two-Dimensional Magnets**, ***Ti Xie,*** *Jierui Liang,* University of Maryland College Park*; Dhritiman Bhattacharya,* Georgetown University*; Hasitha Suriya Arachchige,* University of Tennessee, Knoxville*; Victor Yakovenko,* University of Maryland College Park*; David Mandrus,* University of Tennessee, Knoxville*; Zi Qiang Qiu,* University of California at Berkeley*; Kai Liu,* Georgetown University*; Cheng Gong,* University of Maryland College Park

A magnetic material, while dressed with different spin configurations, can host a variety of emergent phenomena such as chiral domain walls, skyrmions, and Majorana fermions. Traditional preparation of various spin textures in magnetic films by transforming an already established spin pattern demands intensive energy to cause spin flipping or domain wall motion. In contrast, engineering the phase transition kinetics potentially opens up new avenues to achieve desired spin configurations. The two-dimensional (2D) layered magnets, owing to the ultra-thinness, allow the magnetism control by various external stimuli, among which optical approaches promise non-destructive manipulation, both locally and globally. In this talk, I will introduce how we demonstrated a low-power

optical control of 2D magnets. By perturbing the phase transition kinetics, we found that optically excited electrons are multiple orders of magnitudes more effective than electrostatically doped electrons in influencing magnetic domains. Our low-power optical operation paves the new avenue to efficiently engineer 2D spin textures for a plethora of emergent quantum phenomena.

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***, *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 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 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 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 Er^{3+} ions at temperatures ≥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.

2D Materials

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

2D Materials: Devices and Applications

Moderators: Kuan Eng Johson Goh, National University of Singapore, **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 (MoS2, semiconductor) and titanium carbide MXene (Ti3C2, metal) by investigating the temperature, gate and magnetic field dependencies of their electrical conductivity.[7]

Charge transport in printed few-layer MXene and MoS2 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]

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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_2 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_2 (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.

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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_xSe_{2-x}) 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_2 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 WS2 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_2 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_2 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_g) of WS_2 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_g 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_g 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-gown monolayer WS_2 to exhibit an electronic gap of 2.56 eV, larger than 2.43 eV for the mechanically transferred one. The slightly larger E_g 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 WS_2. These findings provide important guidelines for tailoring band alignments for WS_2-based heterostructures and optoelectronic devices.

9:30am **2D+AQS+EM+NS+QS+TF-FrM-6 Atomic Precision Manufacturing for Carbon Nanotube Field Effect Transistors (CNTFETs) for 10X Microelectronics Energy Efficiency***, **Dawei Wang**, Steffen McKearnan,* Carbon Technology Inc.

The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) is leading a multi-organization effort to solve for rapidly growing U.S. computing energy use with its initiative in energy efficiency scaling for two decades (EES2) for microelectronics. Under this initiative, DOE/AMMTO has funded a portfolio of EES2 device technology R&D projects that promise a first >10X energy efficiency increase by 2030. This paper will highlight the most recent of these projects—the use of atomically precise manufacturing techniques to solve carbon nanotube (CNT) device fabrication challenges. Carbon nanotube conduction exceeds that of the best metals by many orders of magnitude. Conduction from Teflon to CNTS varies across 33 orders of magnitude. The size of a human to the universe is only 27 orders. Current semiconductors, even doped, are orders of magnitude worse conductors than CNTs. Because metals are orders of magnitudes better than silicon or GaAs, we metallize them to create circuits. However, copper is close to a million times lower conductivity per atom than a CNT. Even with a double damascene processes, Cu fails due to electromigration at ~1000x the atomic cross-section of a CNT. DOE industry partner Carbon Technology, Inc has pioneered the engineering of atomically precise catalyst particles as small as 10 atoms across. These are used to control CNT diameter in standard chemical vapor deposition CNT synthesis. With diameter control, chiral (semi vs metallic) control becomes a matter of “rusting” the metallic CNTs into CO_2. High quality CNTs on silicon using standard metal contacts and interconnects will provide at least a 10x boost in the efficiency speed trade-off by 2030. In the full EES2 time scale of 20 years, All Carbon Electronics (ACE), semiconducting CNTs interconnected with metallic CNTs (or graphene) on diamond substrates, will deliver the full 1000x performance increase over silicon CMOS and the EES2 vision. With smart investments in carbon, we will stop pounding sand and deliver the diamond age. This talk will present transmission and scanning electron, Raman and Atomic Force microscopy as well as electrical data showing the CNT control needed to deliver on EES2. Simple graphics showing improvement over silicon will also be presented.

9:45am **2D+AQS+EM+NS+QS+TF-FrM-7 The Electronic Band Structure and Conduction Band Formation of $HfSe_3$***, **Gauthami Viswan**[1]*, 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 Universite 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 $HfSe_3$ was investigated with nano-spot angle resolved photoemission spectroscopy (nanoARPES). $HfSe_3$ 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 TiS_3 and ZrS_3 from prior studies.[1] X-ray absorption spectroscopy (XAS) has been used to characterize the unoccupied states of $HfSe_3$ and will be compared to the XAS spectra of HfS_3 [2] and TiS_3 and ZrS_3.[3] 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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10:00am **2D+AQS+EM+NS+QS+TF-FrM-8 Green Synthesis of Pd-Doped 2D Materials for Energy Applications***, Stefania Sciacca,* University of Catania, Catania, Italy*; Cassandra Pichry,* University of Mons, Belgium*; Roberto Fiorenza, Salvatore Scirè, Luisa D'Urso, Carmela Bonaccorso, Giuseppe Forte,* University of Catania, Catania, Italy*; **Cristina Satriano**,* University of Catania, Italy

In this work, we present the preparation and comprehensive physicochemical characterisation of bioinspired nanostructured 2D hybrids based on graphene oxide analogues functionalised with palladium (Pd) nanoparticles, synthesised via a green wet-chemical route. Using glucose as a sustainable reducing agent and polyvinylpyrrolidone (PVP) as a stabilising agent, we achieved controlled deposition of Pd nanoparticles on the 2D surface, ensuring structural integrity and improved dispersion.

The physicochemical properties of the resulting hybrids were thoroughly investigated using X-ray photoelectron spectroscopy (XPS), confocal Raman microscopy, UV-visible absorption and fluorescence spectroscopy analyses to elucidate the chemical and electronic structure. In particular, the ratio of ordered to disordered carbon domains was exploited to gain insight into the structural evolution of the GO-derived materials. This ratio was correlated with the presence of oxygen- and/or sulfur-containing moieties, providing valuable information on the degree of functionalisation and the influence of heteroatom doping on the hybrid structure. Through quantum mechanical calculations, the interaction energy between graphene oxide and the adsorbed palladium nanoparticles was determined, along with the simulation of absorption and Raman spectra generated by this system. Morphological and topographical features were analysed by atomic force microscopy (AFM) and transmission electron microscopy (TEM), revealing uniform nanoparticle distribution and nanoscale hybrid architecture. These Pd-doped 2D hybrids beyond graphene exhibited promising photocatalytic activity, especially in hydrogen (H_2) generation under simulated solar illumination, highlighting their potential in sustainable energy conversion applications.

Acknowledgements: CS and CB acknowledge the financial support by MUR in the framework of PRIN2022-PNRR call under project CoMu4CaT.

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 $Ti_3C_2T_x$ 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]. Laslty, this talk will highlight recent insights into WS_2 nucleation and film growth on sapphire using tungsten hexacarbonyl and

[1] **SSD Morton S. Traum Award Finalist**

hydrogen sulfide precursors in an AIXTRON 2D Close Coupled Showerhead MOCVD 3 × 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 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_2 reduction reaction (CO_2RR). 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_2RR 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**, 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_2 and WS_2 on large area nanostructured samples fabricated by laser interference lithography (either MoS_2 nanostripes arrays or conformal MoS_2 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_2 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_2 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^2-scale) nanoscale reshaping of vdW heterostructures. Specifically, we report a flat-optics platform using vertically stacked WS_2-MoS_2 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 founding 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*f*) 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*f*) 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*f* 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*f* 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*f* reduced to 588 ppm/°C.

A lower TC*f* 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*f* 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.

11:45am **2D+AQS+EM+NS+QS+TF-FrM-15 Nitrogen Doped Graphene Materials for Solid-State Hydrogen Storage***, **Peter Rice**, Buddhika Alupothe Gedara, Mi Yeon Byun,* Pacific Northwest National Laboratory*; Sam Johnson,* Colorado School of Mines, USA*; Maria Sushko, Elizabeth Denis, Zbynek Novotny, Zdenek Dohnalek, Bojana Ginovska, Tom Autrey,* Pacific Northwest National Laboratory

In this work we report our recent experimental and computational findings on controlling the interaction of liquid-organic hydrogen carriers (LOHC's) and hydrogen (H) with nitrogen (N)-doped graphene materials for solid-state H-storage. Specifically, density functional theory (DFT) calculations, inverse gas chromatography (iGC), X-ray photoelectron spectroscopy (XPS)and nuclear magnetic resonance (NMR) are used to quantify both the LOHC (benzene and pyridine) and H adsorption thermodynamics, on materials with varying concentrations of pyridinic and graphitic N. We find that N-doping with basal plane graphitic N has the greatest impact on the LOHC adsorption energetics, compared with basal plane pyridinic and edge site N, due to an enhancement of the π-π stacking configuration. Interestingly, the opposite trend is observed for H adsorption, whereby the calculated adsorption energies and XPS binding energy shifts suggest that pyridinic sites are key sites for binding H, compared with basal plane graphitic N. Our findings provide some guiding principles for developing novel N-doped graphene materials for H_2 storage.

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