Quantum Science and Technology Mini-Symposium
Room 123 - Session QS1+VT-MoM

Vacuum Systems for Quantum Applications

Moderators: Freek Molkenboer, TNO Science and Industry, the Netherlands, **Russell Gleason**, Infleqtion, **Corey Rae McRae**, National Institute of Standard and Technology, **David Pappas**, Rigetti Computing

8:15am **QS1+VT-MoM-1 High-Precision, Four-Way Comparison of Three Cold Atom Vacuum Standards and an Orifice Flow Standard***, **Stephen Eckel**, D. Barker, J. Fedchak, J. Scherschligt,* National Institute of Standards and Technology (NIST)

The cold atom vacuum standard (CAVS) is the first primary standard and sensor for vacuum in the ultra-high vacuum regime and below. By measuring the loss rate of ultra-cold atoms from a conservative magnetic trap, the CAVS infers the pressure of the surrounding vacuum from first principles calculations of the scattering cross section. Various CAVSs have been constructed or are under construction, with different sensor atoms, sizes, and technical capabilities. In 2023, we reported the first comparison of two CAVSs – a laboratory-sized version based on ^{87}Rb and a portable version based on ^{7}Li – to a traditional vacuum metrology apparatus, an orifice flow standard. This initial experiment showed agreement between all three at roughly the 2 % uncertainty level. Here, we report a comparison between three different CAVSs – a laboratory-sized version that can use either ^{7}Li or ^{87}Rb and a portable version that uses ^{7}Li – and our orifice flow standard. We anticipate our new comparison will have total uncertainties < 1 %. In combination with other studies, our results represent a stringent test of quantum mechanical scattering theory.

8:30am **QS1+VT-MoM-2 Vacuum Based Quantum Technology with Aluminum Alloys for Space Applications***, **Klaus Bergner**, F. Löwinger, C. Gruber, L. Gerlach, S. Hüttl, L. Axtmann, A. Trützschler, J. Hertel,* VACOM, Germany*; J. Schneider, L. Kanzenbach, T. Schmidt, S. Wieland, D. Richter,* Fraunhofer Institute for Machine Tools and Forming Technology IWU, Germany*; J. Grosse, M. Warner, M. Elsen,* ZARM Center of Applied Space Technology and Microgravity, Germany

The advancement of quantum technologies has opened new horizons for space applications with capabilities in communication and metrology. This talk explores the potential of vacuum-based quantum technology utilizing aluminum as a pivotal material to enabling access to a wide range of robust and miniaturized turn-key solutions. Vacuum systems used in these quantum physics package solutions often require low form factors, low weight as well as robust and economic design combined with a low magnetic susceptibility and low outgassing rates. But current first demonstrators mainly rely on expensive, bulky, fragile, and unique solutions.

To overcome these limitations, these systems demand the miniaturization as well as increased reliability of used vacuum systems. Optimization and up-scaling of manufacturing processes is key to distinguish competitive technologies for use in commercial applications. One key factor of this approach could be the use of aluminum alloys as base material of vacuum systems. An advantage of aluminum is simpler processing during manufacturing and the associated simpler miniaturization approach. However, the use of aluminum-based ultra-high vacuum (UHV) systems for space applications has not been qualified, nor have the effects of static and dynamic mechanical loads and temperature fluctuations been researched. Due to the complexity of this qualification work, in this joint paper we present the effects of mechanical and thermal influences on the critical system components - the releasable ConFlat (CF) sealing technologies.

The mechanical load of aluminum UHV CF sealing was characterized within a cooperation between Center of Applied Space Technology and Microgravity in Bremen and VACOM. The talk shows results of leakage rate due to static loads. In addition, a disadvantage of aluminum is the temperature limitation of only 120 °C. Within the cooperation between Fraunhofer Institute IWU in Chemnitz and VACOM it was possible to raise this limit up to 200 °C with our newly developed aluminum UHV CF sealing technology. Both results demonstrate the high temperature and mechanical stability of aluminum related CF sealing technology. In summary, this talk is intended to understand the demands of quantum space technology for vacuum systems and allows to develop a proper design of space suitable commercially viable solutions.

8:45am **QS1+VT-MoM-3 Compact UHV Technology for Quantum***, **Alex Kato**,* IonQ **INVITED**

UHV systems for quantum technology (E.g. sensors, computing) can be made smaller by moving away from conventional vacuum parts. I will review several ways in which size, weight, and power can be significantly reduced without sacrificing on desired system performance. This requires moving away from conventional vacuum components, such as off the shelf conflat flanges and windows, feedthroughs, and gauges.

9:15am **QS1+VT-MoM-5 Quantum-Based Sensors and Standards with the NIST on a Chip Program***, **Jay Hendricks**,* NIST*; B. Goldstein,* NIST-Gaithersburg

The NIST on a Chip program (NOAC) is briefly introduced as a forward-looking vision of the future of measurement science.The world-wide redefinition of units that occurred on May 20th, 2019, has opened new ways to think about metrology under a “zero-chain-traceability” paradigm.Next generation quantum-based sensors and standards, based on physical constants of nature, are briefly introduced, for pressure, vacuum, mass and more.The re-definition of the SI units enables new ways to realize the units for the kelvin, mass, and therefore the pascal. A new way to realize the pascal is exciting for vacuum technology (VT), will lead to other exciting applications. These quantum-based systems; however exciting, do raise new challenges and several important questions: Can these new realizations enable the size and scale of the sensor to be miniaturized to the point where it can be imbedded into everyday products?What will be the role of metrology institutes in this new ecosystem of measurement?Where will these new quantum-based systems go and what will they do? This talk will begin to explore these important questions.

9:30am **QS1+VT-MoM-6 3D Printed Ion Traps for Quantum Computation***, **Kristin Beck**,* Lawrence Livermore National Laboratory **INVITED**

Trapped atomic ions are one of the leading qubit candidates for quantum computing. The fidelity of quantum gates and the noise performance of a quantum processor built on this platform depends on the degree of isolation between the classical environment and the ions. One leading noise source is electric field noise. Additive manufacturing has introduced the possibility of generating accurate, replicable and scalable ion traps with geometries that promise to reduce sensitivity to this noise source. In this talk, I will describe miniaturized RF Paul traps that we have fabricated at LLNL using high-resolution 3D printing approach based on two-photon polymerization and share the results of initial tests.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Quantum Science and Technology Mini-Symposium
Room 123 - Session QS2-MoM

Quantum Simulations: Materials, Power Distribution, Computing, and Machine Learning Applications

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

10:30am **QS2-MoM-10 Power System Dynamic Simulation with Generalized Quantum Carleman Linearization***, J. Chen, **Yan Li**,* The Pennsylvania State University **INVITED**

The dynamics of power systems are described by a set of nonlinear differential-algebraic equations (DAEs). Over the past few decades, the expansion of the power system scale has led to a notable increase in the dimension of DAEs, posing a substantial challenge for conventional numerical integration methods to simulate power system dynamics. Herein, we introduce a novel generalized quantum Carleman linearization method to tackle dynamic simulation of large-scale power systems, substantially mitigating computational complexity compared to conventional methods. In light of the characteristics of nonlinear power system DAEs, they are transformed into 4th order inhomogeneous polynomial DAEs through a diffeomorphic transformation. By iteratively employing high-dimensional hyperplanes for approximating nonlinear algebraic equations, the classical ordinary differential equation solver, Carleman linearization, can be extended to solving the high-order DAEs of power systems. Consequently, the proposed method can yield a quantum state proportional to the solution of the DAEs in time O(log (n)), exponentially smaller than the linear complexity of Euler's method. Numerical results demonstrate that the

proposed method can successfully obtain the trajectory of dynamic simulation of power systems with small errors under various scenarios.

11:00am **QS2-MoM-12 Quantum Computer Simulation of Near-Surface Oxygen Vacancies in α-Al_2O_3 (0001)**, ***Vijaya Begum-Hudde***, *Y. Lee,* University of Illinois at Urbana-Champaign*; B. Jones,* IBM*; A. Schleife,* University of Illinois at Urbana-Champaign

Aluminum oxide is a technologically-relevant material as it is employed in a wide range of applications such as catalysis, quantum devices, aviation, and ship industry, among others. Corrosion is a naturally-occurring process in this material, and due to its detrimental effect on the optimal performance, initiation and propagation of corrosion is an area of active research. The near-surface vacancy in the most stable phase, α-Al_2O_3, plays an important role in corrosion, and an improved understanding of the electronic structure is necessary to describe these processes.

We employ first-principles calculations and quantum simulations for an in-depth study of the near-surface O vacancies in α-Al_2O_3 (0001). The geometry of the relaxed Al-terminated pristine (0001) surface obtained with the hybrid exchange-correlation functional (HSE06) are consistent with X-ray diffraction results. Upon introducing an O vacancy, a shallow in-gap electronic defect state. Its band-decomposed charge density and that of the second unoccupied state reveal a strong charge localization near the O vacancy and the adjacent surface Al atom. We study these vacancy states with quantum-defect embedding theory (QDET) calculations to unravel their ground- and excited-state properties. We define an active space consisting of strongly localized states near the defect and treat the remainder as environment. An effective Hamiltonian is solved for the active space which includes the effective screening from the environment within the random phase approximation to obtain the eigenvalues with full configuration interaction (FCI).

Furthermore, we solve the effective Hamiltonian on a quantum computer by employing a model consisting of an active space of one occupied and one unoccupied band from the QDET calculation. On a four-qubit circuit with a Unitary coupled-cluster (UCC-3) ansatz, we calculate the ground-state energy for the active space with the variational quantum eigensolver (VQE). On the noiseless simulator, we achieve excellent agreement with the reference FCI values. Upon introducing noise with a noise model from hardware, the simulator renders an error of 0.19±0.03 eV. We use zero-noise extrapolation with global folding for error mitigation, and successfully reduce the error to 0.01±0.04 eV. Also, a subspace-search VQE implementation to calculate the excited-state eigenvalues for the minimum model results in very good agreement with the first and second excited FCI values.

Funding by the IBM-Illinois Discovery Accelerator Institute is gratefully acknowledged.

11:15am **QS2-MoM-13 Quantum Inception Score: A Quality Measure of Quantum Generative Models**, ***Akira Sone***, University of Massachusetts Boston

This presentation is based on our recent work [arXiv:2311.12163]. One of the most significant areas in quantum machine learning is quantum generative models. These models are a leading strategy for unsupervised learning, which focuses on uncovering hidden patterns in unlabeled data sets and classifying them. The primary goal of generative models is to train a generator to produce data with high accuracy and substantial diversity from a large amount of unlabeled data, reflecting their quality. Here, we focus on the quantum generative models where both the generators and classifiers are fully quantum. We introduce a novel quality measure called the quantum inception score, linking the classical capacity of the quantum channel playing a role as a quantum classifier. We demonstrate that the entanglement output generated by the quantum generator could contribute to further quality enhancement due to the potential superadditivity of the classical capacity. Also, we demonstrate that the quality degradation due to the quantum decoherence can be captured by using the quantum fluctuation theorems. We also show the application of the quantum inception score in the quantum phase classification in the one-dimensional spin-1/2 chain system. Our results underscore the importance of exploring quantum foundations and communication approaches in studying quantum machine learning protocols.

This work is supported by NSF under Grant No. MPS-2328774.

11:30am **QS2-MoM-14 Deep-learning-based Randomness assessment of Quantum Random Number Generators**, ***Hamid Tebyanian***, University of York, UK

Abstract—This paper explores a novel randomness evaluation method for data produced by quantum random number generators (QRNGs), leveraging quantum mechanics to ensure the data's randomness. We employ neural networks and machine learning techniques to analyze the operational principles of QRNGs, enabling the test suites to assess the generators based on their predictability scores. Our findings demonstrate that our model's ability to predict outcomes surpasses that of comparable approaches. Additionally, we discuss the optimal timing for conducting these tests—specifically, analyzing the raw output from QRNGs before processing through an extractor yields the best performance.

Nanoscale Science and Technology
Room 114 - Session NS1+2D+QS-MoA

Functionality in 2D Nanostructures and Devices

Moderator: Dahlia Klein, Weizmann Institute of Science, Israel

1:30pm **NS1+2D+QS-MoA-1 Low-Dimensional Neuromorphic Electronic Materials and Applications**, ***Mark Hersam***, Northwestern University **INVITED**

The exponentially improving performance of digital computers has recently slowed due to the speed and power consumption issues resulting from the von Neumann bottleneck. In contrast, neuromorphic computing aims to circumvent these limitations by spatially co-locating logic and memory in a manner analogous to biological neuronal networks [1]. Beyond reducing power consumption, neuromorphic devices provide efficient architectures for image recognition, machine learning, and artificial intelligence [2]. This talk will explore how low-dimensional nanoelectronic materials enable gate-tunable neuromorphic devices [3]. For example, by utilizing self-aligned, atomically thin heterojunctions, dual-gated Gaussian transistors have been realized, which show tunable anti-ambipolarity for artificial neurons, competitive learning, spiking circuits, and mixed-kernel support vector machines [4,5]. In addition, field-driven defect motion in polycrystalline monolayer MoS_2 enables gate-tunable memristive phenomena that serve as the basis of hybrid memristor/transistor devices (i.e., 'memtransistors') that concurrently provide logic and data storage functions [6]. The planar geometry of memtransistors further allows multiple contacts and dual gating that mimic the behavior of biological systems such as heterosynaptic responses [7]. Moreover, control over polycrystalline grain structure enhances the tunability of potentiation and depression, which enables unsupervised continuous learning in spiking neural networks [8]. Finally, the moiré potential in asymmetric twisted bilayer graphene/hexagonal boron nitride heterostructures gives rise to robust electronic ratchet states. The resulting hysteretic, non-volatile injection of charge carriers enables room-temperature operation of moiré synaptic transistors with diverse bio-realistic neuromorphic functionalities and efficient compute-in-memory designs for low-power artificial intelligence and machine learning hardware [9].

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[7] H.-S. Lee, *et al.*, *Advanced Functional Materials*, **30**, 2003683 (2020).

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2:00pm **NS1+2D+QS-MoA-3 Defect Manipulation in van der Waals Heterostructures and its Applications**, ***Son Le***, Laboratory for Physical Sciences; *T. Mai, M. Munoz, A. Hight Walker, C. Richter,* 100 Bureau Dr.; *A. Hanbicki, A. Friedman,* 8050 Greenmead Dr. **INVITED**

Reliable and accurate spatial doping of 2-dimensional (2D) materials is important for future applications using this novel class of materials. Here, we present our work on photo-doping of an h-BN/Graphene/h-BN heterostructure. Natural defect states in bulk h-BN can remotely dope graphene and can be optically activated or deactivated. In this way, we can modify both the carrier density and type in graphene accurately and reversibly by several orders of magnitude. Using a spatially-resolved light source, we can activate photo-dopants in selected areas of the sample, and by laterally modulating the doping, we have created PNP junction (PNPJ) devices. *In-situ* quantum Hall measurements were used to demonstrate the effectiveness of this doping technique and characterize the electrostatic profile of the PNPJ. Doping and undoping the heterostructure in a specific sequence, we were able to introduce and destroy correlation among the dopants. Defect correlation greatly enhances carrier mobility while the destruction of this correlated state significantly degrades the carrier mobility in the graphene, effectively creating a mobility switch. An elegant demonstration of this mobility switch is the observation of spin and valley-resolved Landau levels of the graphene in the quantum Hall regime with high-mobility, dopant correlated states, and spin and valley -degenerate Landau levels in the low-mobility, dopant uncorrelated states. I will discuss ongoing studies to better understanding the nature of these defects with photo-doping measurements of different hBN thicknesses as well as hBN from different sources. This doping technique opens up the possibility to engineer novel device and expand the applications of 2D heterostructures.

2:30pm **NS1+2D+QS-MoA-5 Extraordinary Tunnel Electroresistance in Layer-by-Layer Engineered Van Der Waals Ferroelectric Tunnel Junctions**, ***Qinqin Wang***, Department of Electrical and Computer Engineering and Quantum Technology Center, University of Maryland, College Park

The ability to engineer potential profiles of multilayered materials is critical for designing high-performance tunneling devices such as ferroelectric tunnel junctions (FTJs). FTJs comprise asymmetric electrodes and a ferroelectric spacer, promising semiconductor platform-compatible logic and memory devices. However, the traditional FTJs consisting of metal/oxide/metal multilayer heterostructures can only exhibit modest tunneling electroresistance (TER, usually $<10^6$), which is fundamentally undermined by the unavoidable defect states and interfacial trap states. Here, we constructed van der Waals (vdW) FTJs by a layered ferroelectric $CuInP_2S_6$ (CIPS) and graphene. Owing to the gigantic ferroelectric modulation of the chemical potentials in graphene by as large as ~1 eV, we demonstrated a giant TER of 10^9. While inserting just a monolayer MoS_2 between CIPS/graphene, the off state is further suppressed, leading to $>10^{10}$ TER. Our discovery opens a new solid-state paradigm where potential profiles can be unprecedentedly engineered in a layer-by-layer fashion, fundamentally strengthening the ability to manipulate electrons' tunneling behaviors and design advanced tunneling devices.

Keywords: 2d materials, ferroelectric tunnel junctions, tunneling electroresistance

2:45pm **NS1+2D+QS-MoA-6 Scanning Tunneling Microscopy Studies of Twisted Transition Metal Dichalcogenides**, ***Adina Luican-Mayer***, STEM 150 Louis Pasteur Private, Canada

Material systems, devices, and circuits, based on the manipulation of individual charges, spins, and photons in solid-state platforms are key for quantum technologies. Two-dimensional (2D) materials present an emerging opportunity for the development of novel quantum technologies, while also pushing the boundaries of fundamental understanding of materials. Our laboratory aims to create quantum functionality in 2D systems by combining fabrication and assembly techniques of 2D layers with atomically precise microscopy.

In this talk, I will focus on experimental observations of novel phenomena in moiré structures created by twisting 2D layers using scanning tunnelling microscopy and spectroscopy. I will discuss the demonstration of reversible local response of domain wall networks using scanning tunneling microscopy in ferroelectric interfaces of marginally twisted WS_2 bilayers. Moreover, in the case of twisted WS_2 bilayers close to 60°, we observe signatures of flat bands and study the influence of atomic relaxation on their band structure.

3:00pm **NS1+2D+QS-MoA-7 Hybrid Molecule/Quantum Material Van Der Waals Heterostructures**, ***Emanuele Orgiu***, Institut National de la Recherche Scientifique (INRS), Canada

The rise of graphene and related 2D materials makes it possible to form heterostructures held together by weak interplanar van der Waals (vdW) interactions. The interactions of such 2D layers with adventitious contaminants is able to exert a strong effect on its major electronic characteristics [1]. However, the controlled incorporation of ordered organic molecules within these systems holds an immense potential. Whilst nature offers a finite number of 2D materials, an almost unlimited variety of molecules can be designed and synthesized with predictable functionalities [2-3]. The possibilities offered by systems in which continuous molecular layers are interfaced with inorganic 2D materials to form hybrid organic/inorganic van der Waals heterostructures are emphasized. Similar to their inorganic counterpart, the hybrid structures have been exploited to put forward novel device architectures. Moreover, specific molecular groups can be employed to modify intrinsic properties and confer new capabilities to 2D materials. This work internds to provide the audience with a brief overview of how molecular self-assembly at the surface of 2D materials can be mastered to achieve precise control over position and density of (molecular) functional groups, paving the way for a new class of hybrid functional. In particular, within such vdW heterostructures, currently assembled by mechanical superposition of different layers, periodic potentials naturally occur at the interface between the 2D materials. These potentials significantly modify the electronic structure of the individual 2D

components within the stack and their alignment, thus offering the possibility to build up hybrid and novel materials with unique properties.

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3:15pm **NS1+2D+QS-MoA-8 Revealing Quantum Functionality of Thin Films by in situ Characterization with Materials Cluster System***, **Wonhee Ko**,* University of Tennessee Knoxville

Achieving unique quantum properties from the nanostructures is a key to realize novel electronic and quantum devices. Thin films of quantum materials are a promising candidate, but the quantum states in these films are highly fragile to the ambient condition and require in situ growth and characterization techniques. With collaboration between several groups in Oak Ridge National Laboratory and University of Tennessee, Knoxville, we built materials cluster system that combines in situ epitaxial film growth and characterization instruments, such as molecular beam epitaxy (MBE), pulsed laser deposition (PLD), angle-resolved photoemission spectroscopy (ARPES), and scanning tunneling microscopy (STM). We used the materials cluster system to grow thin films of topological insulators with MBE and observed lattice and electronic structures in atomic scale with STM and ARPES. Interestingly, we found that the step edges possess Rashba edge states with unique spin texture, which interacts with topological surface states depending on the film thickness. The results demonstrate the potential of materials cluster system to exhibit the unique quantum functionality of thin film materials, which will become a foundation for realizing future quantum devices.

3:30pm **NS1+2D+QS-MoA-9 Functionalized 2D Materials for Sustainable Energy Nanomaterials***, **Nozomi Shirato**,* Argonne National Lab

Advancements in carbon dioxide capturing and reduction (CDR) technology are essential to mitigate greenhouse gas-induced climate changes. Currently, the main challenges of CDRs are economical unviability and poor scalability. The need for next-generation high-performance and cost-effective CDR nanomaterials is paramount. Here, we explore functionalized nanomaterials synthesized on a platinum single crystal for various thermo-catalytic functionalities. We aim to understand the roles of single monolayer thick 2D materials for thermocatalytic performance by harnessing atomic-scale surface imaging capability. Utilizing a low-temperature scanning tunneling microscope (LT-STM) to characterize surfaces at atomic resolution, the fully automated temperature-programmed desorption (TPD) measurements evaluate catalytic performance and repeatability under various conditions. The first-principles-based study supports the results, providing additional fundamental insights into CDR technologies.

Quantum Science and Technology Mini-Symposium
Room 123 - Session QS1+EM+MN+PS-MoA

Materials + Devices for Quantum Systems

Moderators: Parag Banerjee, University of Central Florida, **Jaesung Lee**, University of Central Florida

1:30pm **QS1+EM+MN+PS-MoA-1 Elastic Layered Quantum Materials***, **Jiun-Haw Chu**,* University of Washington **INVITED**

Recently elastic strain has emerged as a powerful tool for probing and controlling quantum materials. By changing chemical bond lengths, elastic strain can modulate electronic structure up to very high energy scale. Additionally, as a second rank tensor, strain enables access to various instabilities associated with different symmetry channels. In this talk, I will discuss several examples of the application of strain to unconventional electronic orderings in van der Waals layered materials, including zigzag antiferromagnetism, charge density waves and excitonic insulators.

2:00pm **QS1+EM+MN+PS-MoA-3 Controllable Extended Defect States in Topological Insulators and Weyl Semimetals***, **Eklavya Thareja**, J. Gayles,* University of South Florida*; I. Vekhter,* Louisiana State University

Over the past decade study of topological materials has emerged as one of the most active areas in condensed matter physics, owing to a wide range of their proposed applications ranging from quantum computing to spintronics. What sets them apart from the materials currently used to build information technology is their robustness to disorder. However, in addition to the immunity of their electronic states against disorder, one needs ways to control the properties of these electronic states in these materials. We show that extended defects such as line defects and planar defects host localized states in Topological Insulators and Weyl Semimetals, which are two common topological materials. These localized states can be manipulated by controlling the scattering at the defects, for example, by using an external magnetic field. This leads to controllable spin accumulation and non-dissipative currents near the defects, due spin-momentum locking. These results bring us closer to functional applications.

2:15pm **QS1+EM+MN+PS-MoA-4 Topological Interfacial State in One-Dimensional h-BN Phononic Waveguide***, Y. Wang, **Sanchaya Pandit**,* University of Nebraska - Lincoln

Artificial topological structures have gained considerable research attention in the fields of photonics, electronics, mechanics, acoustics, and many others, as they promise robust propagation without loss along the edges and interfaces. In this work, we explored the topological states in one-dimensional (1D) phononic waveguides empowered by hexagonal boron nitride (h-BN), a hallmark two-dimensional (2D) material with robust mechanical properties that can support phonon propagation in high frequency regime. First, degenerate trivial and nontrivial topological structures were designed based on the Su-Schrieffer-Heeger (SSH) model. The dispersion engineering was then performed to match the passbands and bandgaps for these two topological structures through optimizing the geometric parameters of the unit cells. An interfacial state emerged when connecting these two sets of unit cells together and forming the 1D waveguide. The topological nature of this interfacial state, immune to structural and material parameter perturbation, was verified with the variation of strain and thickness in the waveguide. The phononic topological state studied here can be further coupled with defect-related quantum emitters in h-BN, opening the door for next-generation hybrid optomechanical circuits.

2:30pm **QS1+EM+MN+PS-MoA-5 Scanning Nano-Optical Imaging of Quantum Materials***, **Guangxin Ni**,* Florida State University

Scanning near-field Nano-Optical imaging is an invaluable resource for exploring new physics of novel quantum materials. Surface plasmon polaritons and other forms of hybrid light-matter polaritons provide new opportunities for advancing this line of inquiry. In particular, nano-polaritonic images obtained with modern scanning nano-infrared tools grant us access into regions of the dispersion relations of various excitations beyond what is attainable with conventional optics. I will discuss this emerging direction of research with two examples from 2D layered quantum materials.

2:45pm **QS1+EM+MN+PS-MoA-6 Engineering of Erbium-Implanted Lithium Niobate Films for Integrated Quantum Applications***, **Souryaya Dutta**,* College of Nanotechnology, Science, and Engineering (CNSE), University at Albany*; A. Kaloyeros, S. Gallis,* College of Nanotechnology, Science, and Engineering (CNSE), University at Albany (UAlbany)

Rare-earth-doped materials have garnered significant attention as material platforms in emerging quantum information and integrated photonic technologies. Concurrently, advances in its nanofabrication processes have unleashed thin film lithium niobate (LN), $LiNbO_3$, as a leading force of research in these technologies, encompassing many outstanding properties in a single material. Leveraging the scalability of ion implantation to integrate rare-earth erbium (Er^{3+}), which emits at 1532 nm, into thin film lithium niobate can enable a plethora of exciting photonic and quantum technologies operating in the telecom C-band. Many of these technologies also rely on coupling via polarization-sensitive photonic structures such as waveguides and optical nanocavities, necessitating fundamental material studies.

Toward this goal, we have conducted an extensive study on the role of implantation and post-implantation processing in minimizing implantation-induced defectivity in *x*-cut thin film LN. By leveraging this, we have demonstrated an ensemble optical linewidth of ~140 GHz of the Er emission at 77 K. Our demonstration showcases the effectiveness of our ion

implantation engineering in producing cutting-edge Er emission linewidth in thin film LN at higher temperatures compared to values reported for diffusion-doped bulk materials at liquid helium temperatures (~3 K). Furthermore, we show that the Er photoluminescence (PL) is highly polarized perpendicular to the *x*-cut LN *c*-axis through a systematic and combinational PL and high-resolution transmission electron microscopy (HRTEM) study. These results indicate that using Er rare-earth emitters in thin film LN, along with their polarization characteristics and related ion implantation engineering, presents a promising opportunity to produce highly luminescent Er-doped LN integrated photonic devices for nanophotonic and quantum applications at telecom wavelengths.

Quantum Science and Technology Mini-Symposium
Room 123 - Session QS2+PS-MoA

Advanced Fabrication and Plasma Techniques for Quantum Applications

Moderators: Angelique Raley, TEL Technology Center America, **Sebastian Engelmann**, IBM T.J. Watson Research Center, **David Pappas**, Rigetti Computing

4:00pm **QS2+PS-MoA-11 High-Rate (>50 nm/hour) Plasma-Enhanced ALD of Superconducting NbxTi1-xN with Substrate Biasing for Quantum Technologies***, **Silke Peeters**, L. Nelissen,* Eindhoven University of Technology, Netherlands*; D. Besprozvannyy,* Oxford Instruments Plasma Technology, UK*; N. Choudhary,* University of Glasgow, UK*; C. Lennon,* Oxford Instruments Plasma Technology, UK*; M. Verheijen,* Eindhoven University of Technology, Netherlands*; M. Powell, L. Bailey,* Oxford Instruments Plasma Technology, UK*; R. Hadfield,* University of Glasgow, UK*; E. Kessels,* Eindhoven University of Technology, Netherlands*; H. Knoops,* Oxford Instruments Plasma Technology, UK

The advancement of a wide range of quantum technologies hinges on improvements in materials and their interfaces. Plasma-enhanced atomic layer deposition (PEALD) enables the growth of high-quality superconducting thin films with atomic-scale control. Scalable integration of PEALD in the diverse field of superconducting quantum device fabrication requires the development of versatile, high-throughput processes.

We demonstrate PEALD of superconducting $Nb_xTi_{1-x}N$ films at a high rate of > 50 nm/hour on the Oxford Instruments PlasmaPro ASP system. The RF-driven remote capacitively coupled plasma (CCP) ALD system with small chamber volume allows for low-damage conditions and short cycle times. The CCP source is combined with RF substrate bias functionality allowing for ion-energy control. The depositions consist of NbN and TiN supercycles using the TBTDEN and TDMAT precursors and an $Ar/H_2/N_2$ plasma at a table temperature of 320 °C.

$Nb_xTi_{1-x}N$ films are prepared with film thicknesses ranging from 5 to 100 nm with < 5 % non-uniformity on a 150 mm diameter wafer. Four-point probe measurements yield low room-temperature resistivities increasing with Nb content from 160 µΩ cm (41 nm TiN) to 284 µΩ cm (25 nm NbN). The films are stoichiometric with a low ~2 at.% O impurity content. Accurate $Nb_xTi_{1-x}N$ composition control through supercycling is demonstrated from x=0 to x=1, with the C content increasing from 10 at.% to 19 at.% and the N content correspondingly decreasing from 40 at.% to 26 at.%. EDX mapping confirms homogeneous mixing of Ti and Nb and XRD reveals all prepared films are fcc polycrystalline. The crystallinity and conductivity of the films can be tuned by RF substrate biasing. TEM imaging of the most conductive 50 nm $Nb_{0.5}Ti_{0.5}N$ film prepared with 90 V bias reveals a disordered polycrystalline film in agreement with XRD, which shows peak broadening beyond 50 V bias.

$Nb_{0.5}Ti_{0.5}N$ films of 5 nm to 100 nm thickness display superconducting transitions at critical temperatures of 3.5 K to 10 K. A high sheet kinetic inductance of 470 pH/sq is found for the 5 nm film prepared with 90 V bias. Superconductivity is also confirmed for all explored compositions and substrate bias voltages. As a result, the film properties can be tailored whilst maintaining the high quality required for quantum applications. The novel ALD configuration negates the need for long plasma exposures to achieve this quality. This tunability and high rate of the $Nb_xTi_{1-x}N$ deposition process puts forward PEALD as a promising technique to tackle material challenges in a wide range of quantum technologies.

4:15pm **QS2+PS-MoA-12 Plasma etch study of NbTiN/αSi/NbTiN Josephson Junctions for Superconducting Digital Loic***, **Yann Canvel**, S. Kundu, V. renaud, A. Pokhrel, D. Lozano, D. Vangoidsenhoven, B. Kennens, A. Walke,* IMEC Belgium*; A. Herr,* IMEC

In the development of next-generation logic devices, an attractive complement to CMOS technology would be to leverage the superconducting technology which operate at a low temperature. Superconducting Digital Logic (SDL) devices are attractive as they are inherently faster and have much less power dissipation than their CMOS counterpart. Although SDL devices have existed for decades now, there have been fundamental challenges to scale down its main components and related interconnects. To provide groundwork for exploring SDL device integration, and a possible hybrid integration of SDL/CMOS circuits, one of the key patterning challenges is the Josephson Junction (JJ) device fabrication. JJ devices are the active devices of SDL technology that can potentially provide computational density, energy efficiency and interconnect bandwidth beyond conventional electronics.

In this communication, an in-depth plasma etch investigation is reported to demonstrate the patterning of high-density junctions with diameters between 210-500nm and CD control of <2% across the 300mm wafer. Using the Reactive Ion etching (RIE) technique, the study has firstly consisted of developing a non-standard NbTiN etch process which enables to pattern the JJ pillars through the Top Electrode (TE) and the αSi barrier, down to the Bottom Electrode (BE) with a precise etch landing control. Subsequent etch processes have then required successive engineering optimization to build up the final device. Some of the main challenges to tackle were the etch residues mitigation, the reduction of oxidized NbTiN interfaces and the final electrical contact with the Top metal. The successful fabrication of high density NbTiN/αSi/NbTiN junctions has offered the first demonstration of a Josephson Junction compatible with CMOS BEOL. Some electrical measurements at room and cryogenic temperatures will complete the investigation by showing high critical current, high speed and device stability up to 420°C.

Pokhrel, A *et al.,* First Demonstration of High Density NbTiN/αSi/NbTiN Josephson Junctions. *IEEE Symposium on VLSI Technology & Circuits (VLSI), (2024).*

Pokhrel, A. *et al.* Towards Enabling Two Metal Level Semi-Damascene Interconnects for Superconducting Digital Logic: Fabrication, Characterization and Electrical Measurements of Superconducting $Nb_xTi_{(1-x)}N$. *IEEE International Interconnect Technology Conference (IITC)*, (2023).

Holmes, D. S. *et al.* Energy-Efficient Superconducting Computing - Power Budgets and Requirements. *IEEE Transactions on Applied Superconductivity* **23**, 1701610–1701610 (2013).

Herr, Q. P. *et al.* Ultra-low-power superconductor logic. *Journal of Applied Physics* **109**, 103903 (2011).

4:30pm **QS2+PS-MoA-13 Patterning Improvements and Oxidation Mitigation of $Nb_xTi_{(1-x)}N$ Metal Lines Processes for Superconducting Digital Logic***, **Vincent Renaud**, Y. Canvel, A. Pokhrel, S. Iraci, M. Kim, B. Huet, J. Soulie, S. Sarkar, Q. Herr, A. Herr, Z. Tokei,* IMEC, Belgium

One promising alternative to standard CMOS technology is Superconducting Digital Logic (SDL) which enables computing at cryogenic temperature and, thus, performs faster at a reduced cost and power. Recently, it was demonstrated that a two-metal level BEOL unit process using $Nb_xTi_{(1-x)}N$ for the metal lines with a critical dimension of 50nm could be achieved on 300mm wafers. Cryogenic temperature electrical measurement showed that the lines and via of the device have a critical temperature of 12-13.4 K and a critical current density of 80-113 $mA/\mu m^2$. It was also highlighted that one of the crucial challenge in the making of this technology was the oxidation of the $Nb_xTi_{(1-x)}N$ metal lines during the direct metal etch process of the material itself and/or during the conception of the full device. This oxidation negatively impacts the electrical performance of the wire and could become a serious showstopper for the scalability of the device.

The goal of this study is to discuss different approaches for constructing and patterning the $Nb_xTi_{(1-x)}N$ metal lines while mitigating the oxidation of the device during the process. Different Hard-Mask (HM) materials have been investigated, as well as alternative HM removal processes. Finally, an in-situ

encapsulation of the $Nb_xTi_{(1-x)}N$ metal lines post-etch process has been experimented to mitigate the oxidation the device when exposed to the air or during the sub-sequent dielectric gap-fill. These experiments were coupled with electrical measurements at room and cryogenic temperature with the aim of validating the best fabrication process for the $Nb_xTi_{(1-x)}N$ metal lines for SDL devices.

Pokhrel, A. *et al.* Towards Enabling Two Metal Level Semi-Damascene Interconnects for Superconducting Digital Logic: Fabrication, Characterization and Electrical Measurements of Superconducting $Nb_xTi_{(1-x)}N$. *IEEE International Interconnect Technology Conference (IITC)*, (2023).

Holmes, D. S. *et al.* Energy-Efficient Superconducting Computing - Power Budgets and Requirements. *IEEE Transactions on Applied Superconductivity* **23**, 1701610–1701610 (2013).

Herr, Q. P. *et al.* Ultra-low-power superconductor logic. *Journal of Applied Physics* **109**, 103903 (2011).

4:45pm **QS2+PS-MoA-14 Patterning of TiN and TaN for advanced superconducting BEOL**, ***Thibaut Chêne***, CEA-LETI, France; *R. Segaud, F. Nemouchi, S. Minoret,* CEA-Leti, France; *F. Gustavo,* CEA INP Grenoble, IRIG, France; *J. Garrione, T. Chevolleau,* CEA-Leti, France

The development of new quantum technologies based on superconducting Qubits or spin Qubits becomes a major subject of interest for applications in communication and data computing. Such technology operating at low temperature requires a superconducting rooting development.

The superconducting materials have been selected based on their superconducting properties and their integration capabilities in an industrial process flow. The integration is based on a top down approach by patterning successively both metals with a selective etch process to define lines and vias.

To develop the patterning process, a 40 nm thick film of TiN or TaN is deposited by PVD on a SiO_2 layer over 300 mm silicon wafers. Then the lithography is performed on a 193nm stepper to achieve 150 nm line and via critical dimension (CD). Etching developments are carried out on a 300 mm industrial ICP chamber using Cl_2 chemistry with or without HBr or CH_4 addition. A parametric study of Cl_2 based chemistries is performed to achieve a straight profile with low CDbias and also to determine the selectivity of TaN over TiN. Optical Emission Spectroscopy (OES) and quasi in-situ Xray Photo-electon Spectroscopy (XPS) are conducted to better understand the etching mechanisms.

Regarding the TiN, straight profiles and good CD control are achieved with Cl_2/HBr chemistries but micromasking is observed. The micromasking phenomenon will be further discussed in terms of plasma/surface interaction based on the quasi in-situ XPS analyses. The addition of CH_4 instead of HBr prevents the micromasking while keeping a rather straight profile with an etch rate of 70 nm/min. For the TaN, whatever the etching chemistries, lower etch rates are observed in comparison with TiN. This trend is attributed to a higher Ta-N binding energy and lower etch by-product volatility. The Cl_2/HBr and Cl_2/Ar plasma chemistries lead both to CD loss and tapered profile mainly due to a lack of selectivity with the PR. Oppositely, the Cl_2/CH_4 chemistry allows achieving straight TaN profile by adjusting the amount of CH_4. The patterning of 80 nm vias for both TiN and TaN are obtained by combining resist trimming and the etching processes previously optimized for the narrow lines. After this patterning process optimization, the T_c of 150 nm CD structures is measured using a specific test vehicle for both TiN and TaN thin films. We will then leverage the TiN:TaN etching selectivity of 4.6 achieved by tuning the Cl_2/CH_4 amount to integrate TiN vias on TaN lines.

5:00pm **QS2+PS-MoA-15 Optimization of Superconducting Transition Metal Nitride Films Deposited by Reactive High-Power Impulse Magnetron Sputtering**, ***Hudson Horne***, *C. Hugo, B. Reid, D. Santavicca,* University of North Florida

Ultra-thin films of transition metal nitrides are used to create superconducting devices such as superconducting nanowire single-photon detectors, kinetic inductance detectors, and parametric amplifiers. Nanowires made from such materials also have applications in quantum computing, for example as high-impedance, low-dissipation shunts to suppress charge noise in superconducting qubits. In this work, we explore the use of high-power impulse magnetron sputtering (HiPIMS) to optimize the superconducting properties of transition metal nitride thin films for such device applications.

Initial work has focused on niobium nitride deposited using a reactive process in which a niobium target is sputtered in the presence of nitrogen gas. We compare films deposited on silicon substrates via HiPIMS and conventional DC sputtering, and we find that HiPIMS can produce films of the same thickness with a higher critical temperature and a lower normal-state resistivity. Film composition and structure are characterized with scanning electron microscopy, wavelength-dispersive x-ray spectroscopy, and x-ray diffraction, and these results are correlated with the electrical properties of both unpatterned films and nanowires. These characterizations suggest that the improved superconducting properties of the HiPIMS films is the result of optimizing the stoichiometry in the desired δ crystal phase. We show that further improvement in the critical temperature is possible through the use of an aluminum nitride buffer layer and through substrate heating.

We have begun extending these studies to other materials such as titanium nitride and hafnium nitride. This work seeks to systematically explore the HiPIMS process for optimizing transition metal nitride films with an emphasis on ultra-thin films for quantum device applications.

This work was supported by the National Science Foundation through grants ECCS-2000778 and ECCS-2117007.

2D Materials

Room 122 - Session 2D+AP+EM+QS+SS+TF-TuM

2D Materials: Synthesis and Processing

Moderators: Jyoti Katoch, Carnegie Mellon University, **Huamin Li**, University at Buffalo-SUNY

8:00am **2D+AP+EM+QS+SS+TF-TuM-1 Tailored Growth of Transition Metal Dichalcogenides Monolayers and Their Heterostructures*, Andrey Turchanin,*** Friedrich Schiller University Jena, Germany **INVITED**

Two-dimensional materials (2D), their van der Waals and lateral heterostructures possess a manifold of unique electronic, optoelectronic and photonic properties which make them highly interesting for fundamental studies and technological applications. To realize this potential, their tailored growth as well as understanding of the role of their intrinsic defects and 2D-material/substrate interactions are decisive. In this talk, I will present an overview of our recent progress on the synthesis by chemical vapor deposition (CVD), material characterization and studying of fundamental electronic and photonic properties of 2D transition metal dichalcogenide (TMDs) including some applications in electronic and optoelectronic device as well as observing of new excitonic phenomena. A particular focus will be on the lateral heterostructures of TMD monolayers with atomically sharp boundaries and Janus TMDs.

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8:30am **2D+AP+EM+QS+SS+TF-TuM-3 High-Coverage MoS_2 Growth by Two-Step Annealing Process*, Shinichi Tanabe,*** *H. Miura,* Tokyo Electron Ltd., Japan*; N. Okada, T. Irisawa,* AIST, Japan*; Y. Huang, H. Warashina, A. Fukazawa, H. Maehara,* Tokyo Electron Ltd., Japan

Continuation of Moore's Law scaling requires thin channels in nanosheet field-effect transistor architecture. In this respect, transition-metal dichalcogenides (TMDs) are candidates for the channel material because TMDs are expected to show higher mobility than Si when thickness of the channel is extremely thin. Compatibility to Si nanosheet field-effect transistor fabrication process requires TMD/buffer multilayer film. To obtain such film, alternative preparation of TMD and buffer layers is necessary. Although high-quality TMD can be obtained on a buffer layer by transferring TMD from other substrates, development of a reliable transferring method is challenging. Thus, direct growth of a TMD on a buffer layer is preferable.

We report on a successful growth of high-coverage MoS_2 on SiO_2/Si substrate. The process starts with growing an initial film on SiO_2/Si substrate. Here, a continuous initial film can be easily grown by this process with high growth rate. Next, the initial film is sulfurized by a first annealing step followed by crystallization of the film by a second annealing step. The obtained film is a continuous layered film which was confirmed by cross-sectional TEM images. In addition, typical Raman spectra consisted of E_{2g} and A_{1g} peaks are observed in entire substrate which shows that MoS_2 is grown with high coverage. The difference of E_{2g} and A_{1g} peaks is about 21 cm^{-1}. These results indicate that the two-step annealing process is suitable for obtaining MoS_2 in large area.

8:45am **2D+AP+EM+QS+SS+TF-TuM-4 Anomalous Isotope Effect on the Optical Bandgap in a Monolayer Transition Metal Dichalcogenide Semiconductor*, Kai Xiao,*** Center for Nanophase and Materials Sciences Oak Ridge National Laboratory*; Y. Yu,* School of Physics and Technology, Wuhan University, China*; V. Turkowski,* Department of Physics, University of Central Florida*; J. Hachtel,* Center for nanophase and Materials Sciences Oak Ridge National Laboratory*; A. Puretzky, A. Ievlev, C. Rouleau, D. Geohegan,* Center for Nanophase and Materials Sciences Oak Ridge National Laboratory

Isotope effects on optical properties of atomically thin 2D materials have rarely been studied to date due to significant challenges posed by sample-to-sample variations resulting from defects, strain, and substrate interactions, complicating the interpretation of optical spectroscopic results. Here, we report a novel two-step chemical vapor deposition method to synthesize isotopic lateral junctions of MoS2, comprising monolayer single crystals with distinct isotopic regions. This method allowed the minimization of shifts in photoluminescence due to synthetic heterogeneities necessary to confirm the intrinsic isotope effect on the optical band gap of 2D materials. Raman measurements and temperature-dependent photoluminescence spectra revealed an unusual 13 (± 7) meV redshift as the Mo isotope mass increased in monolayer MoS2. This shift is distinct from the trend observed in conventional semiconductors and quantum wells (Si, GaAs, diamond, hBN, etc.). Our experimental characterization, along with time-dependent density-functional theory (TDDFT) and many-body second-order perturbation theory, disclosed that this anomalous shift in the optical band gap in 2D MoS2resulted from significant changes in the exciton binding energy induced by strong exciton-phonon scattering. This study provides fundamental insights into understanding the effect of exciton-phonon scattering on the optoelectronic properties of atomically thin 2D materials.

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.

9:00am **2D+AP+EM+QS+SS+TF-TuM-5 CVD Growth and Characterization of High-Quality Janus SeMoS and SeWS Monolayers*, Julian Picker,*** Friedrich Schiller University Jena, Germany*; M. Ghorbani-Asl,* Helmholtz Zentrum Dresden-Rossendorf, Germany*; M. Schaal, O. Meißner, F. Otto, M. Gruenewald, C. Neumann, A. George,* Friedrich Schiller University Jena, Germany*; S. Kretschmer,* Helmholtz Zentrum Dresden-Rossendorf, Germany*; T. Fritz,* Friedrich Schiller University Jena, Germany*; A. Krasheninnikov,* Helmholtz Zentrum Dresden-Rossendorf, Germany*; A. Turchanin,* Friedrich Schiller University Jena, Germany

Structural symmetry breaking of two dimensional (2D) materials leads to novel physical phenomena. For 2D transition metal dichalcogenides (TMDs) such symmetry breaking can be achieved by exchange of one chalcogen layer with another one. The resulting, so-called Janus TMD structure exhibits an intrinsic dipole moment due to the different electronegativity values of the top and bottom chalcogen layers. Since Janus TMDs do not exist as bulk crystals, they cannot be obtained by exfoliation and need to be synthesized. Recently, we developed a route to grow Janus SeMoS monolayers (MLs) by chemical vapor deposition (CVD). [1] In this approach $MoSe_2$ monolayers are firstly grown on Au foils and then sulfurized to exchange the bottom selenium layer with sulfur atoms. The formation of high-quality Janus SeMoS MLs and the growth mechanism are proven by Raman and X-ray photoelectron spectroscopy (XPS), photoluminescence measurements, transmission electron microscopy and density functional theory (DFT). Here we present an investigation down to the atomic scale of Janus SeMoS MLs grown on Au(111). From low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) measurements we determine experimentally the lattice parameters of Janus SeMoS for the first time. The obtained results are in good agreement with the respective DFT calculation. Based on the angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) study, we also obtain the spin-orbit splitting value of the valence band at the K point. Moreover, applying the same approach, we grow and characterize Janus SeWS MLs and provide a comparative analysis with the Janus SeMoS system.

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9:15am **2D+AP+EM+QS+SS+TF-TuM-6 Location-Selective CVD Synthesis of Circular MoS_2 Flakes with Ultrahigh Field-Effect Mobility**, ***Chu-Te Chen**, A. Cabanillas, A. Ahmed, A. Butler, Y. Fu, H. Hui, A. Chakravarty, H. Zeng,* University at Buffalo-SUNY*; A. Yadav,* Applied Materials, Inc.*; H. Li,* University at Buffalo-SUNY*; K. Wong,* Applied Materials, Inc.*; F. Yao,* University at Buffalo-SUNY

Two-dimensional (2D) semiconducting transition metal dichalcogenides (TMDs) have been considered as promising channel material candidates for future nanoelectronics. The device performance has been significantly improved over the years due to the advancements in understanding of TMD materials, device design, and fabrication process. Despite the early success in demonstrating proof-of-concept devices, scalable and single-crystal growth of TMD films on suitable substrates remains a formidable roadblock to the development of commercially viable TMD-based nanoelectronics. To mitigate this problem, we exploit a controlled growth of high-quality TMD layers at desired locations and demonstrate excellent and consistent electronic properties in transistor device architectures. Taking MoS2 as an example, we develop a precursor-seeded growth strategy for the direct and site-specific synthesis on SiO2 substrates using chemical vapor deposition (CVD). By employing electron-beam lithography to pattern seed layers, precise nucleation and growth at designated positions are achieved. Through systematic exploration of CVD synthesis parameters, ordered arrays of circular MoS2 flakes are successfully grown with the MoO3 seeds serving as the nucleation sites. A comprehensive suite of microscopic/spectroscopic characterizations along with electrical measurements is utilized to analyze the microstructural and transport properties of the as-grown MoS2 flakes. The tri-layer circular MoS2 arrays possess an adjustable and uniform size and exhibit a consistent field-effect mobility up to ~20 cm2/V·s with Bi/Au electrode contacts. These findings showcase a technological breakthrough to 2D material synthesis and hold great promise for future integration of 2D materials in the next generation nanoelectronics.

9:30am **2D+AP+EM+QS+SS+TF-TuM-7 Optoelectronic Properties of Exfoliated and CVD Grown TMD Heterostructures**, ***Elycia Wright**, K. Johnson, S. Coye, M. Senevirathna, M. Williams,* Clark Atlanta University

Transition metal dichalcogenides (TMDs) have attracted significant attention due to their distinctive electronic band structures, which result in intriguing optoelectronic and magnetic properties such as direct bandgap in the visible-infrared range, large exciton binding energies and the presence of two intrinsic valley-contrasting quantities-the Berry curvature and the orbital magnetic moment. Researchers have recently shown interest in studying heterostructures made from different TMD materials. The idea is to combine these materials to create synergistic effects, which can result in even more exciting properties than those found in individual TMDs. For instance, MoS_2/WS_2 heterostructure can exhibit novel and enhanced optoelectronic performances, including bipolar doping and photovoltaic properties. TMD-based heterostructures may open many possibilities for discovering new physics and developing novel applications. While the science of TMDs and TMD-based heterostructures has made significant strides over the past decade, the field has not yet matured. Numerous challenges, particularly in realizing TMD-based practical applications, remain unresolved. This underscores the importance of our collective efforts in pushing the boundaries of this field.

Exfoliation is a common method for assembling TMD heterostructures, but it has limitations in producing TMD heterostructures on a large scale. The chemical vapor deposition (CVD) method can be used to grow TMD heterostructures on a large scale, which is required in massive device production. However, there are numerous challenges in growing high-quality TMD heterostructures with large areas by CVD, which need to be solved before TMD-based practical applications can be achieved. Our research will focus on the growth of heterostructures (MoS_2/WS_2) on various substrates (such as sapphire and SiO_2/Si) using chemical vapor deposition (CVD). We will explore different mechanisms to achieve large area heterostructures and compare the resulting optoelectronic properties with exfoliated heterostructures. The properties will be characterized using Raman and Fourier Transform infra-red (FTIR) spectroscopy and confocal laser optical microscopy.

9:45am **2D+AP+EM+QS+SS+TF-TuM-8 Pulsed Laser Deposited Amorphous Boron Nitride for 2D Materials Encapsulation**, ***Daniel T. Yimam**, S. Harris, A. Puretzky, I. Vlassiouk, G. Eres, K. Xiao, D. Geohegan,* Oak Ridge National Laboratory, USA

Recent advancements in 2D materials have opened new avenues in optoelectronics and microelectronics. However, their integration is hindered by challenges related to materials stability and degradation. Realizing the full potential of 2D materials requires synthesizing and functionalizing an encapsulation layer with desired properties. Recently amorphous boron nitride (aBN) has attracted attention as an ideal low-k material suitable for 2D electronics due to its effectiveness as a protective encapsulation layer.Unlike hexagonal boron nitride (h-BN), which requires high temperatures for deposition and poses challenges for large-area synthesis and integration, aBN can be deposited at significantly lower temperatures. This property makes aBN highly attractive and compatible for back-end-of-line (BEOL) processes in the semiconductor industry.

In this work, we demonstrate that pulsed laser deposition (PLD) enables the deposition of aBN with precise kinetic energy control of precursors, facilitating direct deposition onto 2D materials without significant defect formation. Various in situ plume diagnostics and monitoring tools during deposition were utilized to identify optimal deposition conditions, ensuring ideal kinetic energy ranges and accurate thickness control. This enhances the aBN as an effective encapsulation and barrier against 2D materials thermal degradation, while improving photoluminescence of encapsulated 2D materials. We believe our work significantly impacts future microelectronics by providing low thermal budget method for encapsulating 2D materials and understanding strain and defect evolution. Our work not only advances the practical applications of 2D materials but also paves the way for in situ experimental analysis and diagnostics in the field of material 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, Amorphous Boron Nitride, 2D Materials, Encapsulation, In Situ Diagnostics.

11:00am **2D+AP+EM+QS+SS+TF-TuM-13 Topotaxy for Compositional Variations of Transition Metal Dichalcogenides**, ***Matthias Batzill**,* University of South Florida

Topotaxy is a kind of solid-state reaction in which the product crystal is crystallographically related to the initial crystal. In 2D materials the initial crystal could be a single sheet or a few layers that are being reacted with same or dissimilar elements to produce novel 2D materials that may not exist in the bulk. Here we investigate such topotactical reactions for transition metal dichalcogenides (TMDs) by reacting them with vapor deposited transition metals. This can result in phase transformations of know layered materials, such as $PtTe_2$ +Pt => Pt_2Te_2 [1], new phases such as mirror twin grain boundary networks in $MoSe_2$ or $MoTe_2$ [2], or covalently linking bi-layer TMDs by intercalants of the same or different TMs [3]. The studies are performed on MBE grown TMDs and are further modified by post-growth reaction with TM. The resulting structures are characterized by surface probes, such as STM, photoemission, and LEED. In general, the open structure of many 2D materials make them ideal for topotaxy and provide an approach for modifying their composition and induce new properties. Moreover, it allows to locally modify an extended 2D sheet and thus produce in-plane heterojunctions between 'original' and modified 2D domains in a first step to create in-plane device structures.

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Formation of In-Plane Semiconductor–Metal Contacts in 2D Platinum Telluride by Converting PtTe2 to Pt2Te2.

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2D Materials by Design: Intercalation of Cr or Mn between two VSe2 van der Waals Layers.

Nano Letters 23, 9579-9586 (2023)

11:15am **2D+AP+EM+QS+SS+TF-TuM-14 Solid State Reaction Epitaxy to Create van der Waals Heterostructures between Topological Insulators and Transition Metal Chalcogenides**, ***Salma Khatun***, *O. Alanwoko, V. Pathirage, M. Batzill,* University of South Florida

Van der Waals (vdW) heterostructures have emerged as a promising avenue for exploring various quantum phenomena. However, the formation of these heterostructures directly is complicated, as individual materials could have different growth temperatures, and alloying can occur at the interface. We present an alternative process akin to a solid-state reaction to modify the surface layer of quantum materials and introduce new properties. Specifically, we used vapor-deposited transition metals (TMs), Cr and Mn, with the goal to react with Bi_2Se_3 and transform the surface layer into XBi_2Se_4 (X = Cr, Mn). Our results demonstrate that the TMs have a high selenium affinity that drives Se diffusion toward the TM. We found that when a monolayer of Cr is evaporated, the surface Bi_2Se_3 is reduced to Bi_2-layer, and a stable (pseudo) 2D $Cr_{1+\delta}Se_2$ layer is formed, whereas $MnBi_2Se_4$ phase is formed with a mild annealing for monolayer amount of Mn deposition.[1] However, this phase only occurs for a precise amount of initial Mn deposition. Sub-monolayer amounts dissolve into the bulk, and multilayers form stable MnSe adlayers. Our study highlights the delicate energy balance between adlayers and desired surface-modified layers that govern the interface reactions.[1] The success of obtaining the $MnBi_2Se_4$ septuple layer manifests a promising approach for engineering other multicomponent vdW materials by surface reactions.

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[1] S. Khatun, O. Alanwoko, V. Pathirage, C. C. de Oliveira, R. M. Tromer, P. A. S. Autreto, D. S. Galvao, and M. Batzill,*Adv. Funct. Mater.* **2024**, 2315112

11:30am **2D+AP+EM+QS+SS+TF-TuM-15 AVS National Student Award Finalist Talk: Quasi-Van Der Waals Epitaxial Growth of Thin γ'-Gase Films**, ***Mingyu Yu***[1], University of Delaware*; S. Law,* Pennsylvania State University

As an advanced two-dimensional (2D) layered semiconductor, GaSe has various appealing properties, such as rare intrinsic p-type conductivity, nonlinear optical behavior, high transparency in 650-180000nm, and a shift from an indirect-bandgap single-layer film to a direct-bandgap bulk material. These features make GaSe rich in potential in quantum photonic devices, field-effect transistors, photodetectors, etc. GaSe has a hexagonal crystal structure composed of Se-Ga-Ga-Se quadruple layers (QLs). Each QL is bonded by weak van der Waals (vdW) forces, enabling multiple polymorphs: ε-(2H), β-(2R), δ-(4H), and γ-(3R). They have identical non-centrosymmetric QL with a D_{3h} space group. Besides the four extensively explored polymorphs, a new polymorph, γ'-(3-R) GaSe, was proposed for the first time in 2018. γ'-GaSe is unique for its centrosymmetric D_{3d} QL (Fig. S1), for which γ'-GaSe is predicted to show intriguing properties compared to other polymorphs. However, there are few existing reports on the observation of γ'-GaSe due to its less-favorable formation energy. Moreover, the wafer-scale production of pure GaSe single crystal thin films remains challenging because of the coexistence of stable multiphases and polymorphs.

We developed a quasi-vdW epitaxial growth method to obtain high-quality pure γ'-GaSe nanometer-thick films on GaAs(111)B at a wafer scale. It results in GaSe thin films exhibiting a smooth surface with a root-mean-square roughness as low as 7.2 Å (Fig. S2a) and a strong epitaxial relationship with the substrate (Fig. S2b). More interestingly, we observed a pure γ'-polymorph using scanning transmission electron microscopy (Fig. S2c,d). Through density-functional theory analysis (Fig. S3), γ'-GaSe can be stabilized by Ga vacancies since its formation enthalpy tends to become lower than that of other polymorphs when Ga vacancies increase. We also observed that, unlike other GaSe polymorphs, γ'-GaSe is inactive in room-temperature photoluminescence tests. This may be related to its centrosymmetric QL structure, which we are exploring further. Meanwhile, we systematically studied the growth window for GaSe with high structural quality and identified that GaAs(111)B is more suitable than c-sapphire as a substrate for GaSe growth. Overall, this study advances the wafer-scale production of γ'-GaSe films, and elucidates a method for direct epitaxial growth of hybrid 2D/3D heterostructures with atomically sharp interfaces, facilitating the development of heterogeneous integration. In the future, we will focus on developing the properties and applications of γ'-GaSe, and delving into the understanding of the epitaxial growth mechanism.

11:45am **2D+AP+EM+QS+SS+TF-TuM-16 Investigation of Dry Transfer of Epitaxial Graphene from SiC(0001)**, ***Jenifer Hajzus***, *D. Pennachio, S. Mack, R. Myers-Ward,* U.S. Naval Research Laboratory

Transfer of high-quality graphene from its growth substrate to substrates of technological interest can be necessary to enable its use in certain applications, however it remains challenging to achieve large-area transfer of graphene that is clean and intact. This work utilizes a dry transfer technique in which an adhesive metal stressor film is used to exfoliate epitaxial graphene (EG) from SiC(0001) [1]. In this method, the strain energy in the metal film must be high enough to allow for uniform exfoliation, but low enough such that self-exfoliation of graphene does not occur.

We investigate the dry transfer of monolayer EG (MEG) and hydrogen-intercalated, quasi-freestanding bilayer graphene (QFBEG) grown by sublimation of Si from nominally on-axis 6H-SiC(0001) in a CVD reactor in Ar ambient. A magnetron sputtered Ni stressor layer is used to exfoliate EG and transfer to GaAs, glass, and SiO_2/Si substrates. The Ar pressure during sputtering is found to impact the stress, film density, and roughness of the Ni film, as determined from wafer curvature and X-ray reflectivity (XRR) measurements. By using appropriate sputtering conditions, the Ni/graphene film exfoliates from the entire area of the SiC substrate with use of thermal release tape. Atomic force microscopy (AFM), scanning electron microscopy, Raman spectroscopy, x-ray photoelectron spectroscopy (XPS), and Nomarski microscopy are used to characterize the graphene. The Ni 2p peak was not detected in XPS of the transferred graphene after removal of the Ni film by etching in acid. Additionally, XPS revealed minimal oxide present at the graphene-GaAs interface, consistent with previous reports for this dry transfer method [2].

Raman spectroscopy mapping showed that predominately monolayer graphene is transferred from MEG, while predominately bilayer graphene is transferred from QFBEG. Raman spectroscopy of the SiC substrate after MEG exfoliation shows the $6\sqrt{3}$ buffer layer that forms during growth on SiC(0001) remains on the SiC substrate. Consequently, if there are regions of exposed $6\sqrt{3}$ buffer layer in the as-grown MEG on SiC, AFM shows that there are corresponding gaps in the transferred graphene film where the areas of exposed buffer layer do not transfer. The $6\sqrt{3}$ buffer layer is not present in QFBEG due to the hydrogen-intercalation process. It is found that the same Ni sputtering conditions that led to uniform exfoliation and transfer of MEG result in micron-scale tears in the Ni/QFBEG film. By lowering the strain energy in the sputtered Ni film, these tears can be reduced or eliminated.

[1] Kim, J., *et al.*, Science, 342, 833 (2013).

[2] Kim, H., *et al.*, ACS Nano, 15, 10587 (2021).

Quantum Science and Technology Mini-Symposium
Room 123 - Session QS-TuM

Superconducting Qubits and Surface Engineering for Quantum Applications

Moderators: David Pappas, Rigetti Computing, **Corey Rae McRae**, National Institute of Standard and Technology, **Ekta Bhatia**, NY CREATES, **Sisira Kanhirathingal**, Rigetti Computing

8:00am **QS-TuM-1 Cryogenic Growth of Tantalum on Silicon and the Effect of Substrate Preparation on Superconducting Circuit Performance**, ***Teun van Schijndel***, University of California Santa Barbara*; A. McFadden,* NIST-Boulder*; W. Yánez-Parreño, J. Dong,* University of California Santa Barbara*; R. Simmonds,* NIST-Boulder*; C. Palmstrøm,* University of California Santa Barbara

Recent advances in superconducting quantum information systems show the effectiveness of tantalum as a superconducting material, with qubits reaching coherence times up to 0.5 ms[1,2]. The growth of alpha-Ta is required for the realization of desirable superconducting properties. However, challenges persist as various sources of energy losses arise from material-related factors. One of the potential sources comes from the substrate-superconductor interface. Here, we demonstrate cryogenic growth (< 20 K) of polycrystalline alpha-Ta on silicon substrates. First, we show the ability to grow alpha-Ta on different substrate orientations and confirm with X-ray diffraction and transport that we form a similar polycrystalline-oriented film regardless of the substrate orientation. Furthermore, we explore different substrate preparation techniques such as HF etching and *in-situ* Atomic Hydrogen Annealing. We will study the silicon substrates before growth by *in-situ* Scanning Tunneling Microscopy (STM).

[1] **AVS National Student Award Finalist**

Next, we perform microwave measurements on fabricated CPW resonator circuits and 2D Transmon qubits and compare the performance of different surface orientations and substrate preparation techniques. We aim to correlate the findings in the microwave measurements with our observations in STM.

1) Place, A.P.M., *et al.*, *Nat Commun* **12**, 1779 (2021).

2) Wang, C., *et al.*, *npj Quantum Inf* **8**, 3 (2022).

Supported by ARO W911NF2210052 and UCB NSF Quantum Foundry funded via the Q-AMASE-i program under award DMR-1906325

8:15am **QS-TuM-2 Thin Film Growth of Alpha- and Beta-Ta on Low-Loss Oxides for Superconducting Resonator Development***, N. Price, C. Wade, L. Don Manuwelge Don,* Miami University*; S. Padhye, H. Yusuf, E. Mikheev,* University of Cincinnati*;* ***Joseph Perry Corbett****,* Miami University

Superconducting qubits are one of the leading candidates for creating quantum computers with the potential to surpass modern supercomputers in solving specific problems. Steady progress over the last 20 years has occurred, increasing the lifetime of quantum states and the number of qubits. A popular method to create a 2-level quantum system for quantum computation is to pattern a low-loss insulator/superconductor heterostructure into circuits. A recent new discovery in the qubit community is the fabrication of qubits from α-Ta thin films with improved coherence times of 0.5 ms! Despite recent success, an impetus for fundamental material science on insulator/superconductor heterostructure is well-recognized in the QISE community. We perform a systematic investigation of the nucleation and thin film microstructure of alpha- and beta-Ta grown on several low-dissipation insulating oxide substrates alongside identifying essential growth conditions that result in material conditions that adversely affect the sharpness of superconducting transition and Q-factor. Utilizing a combination of coil-assisted sputtering epitaxy, electron and scanning probe microscopy, alongside millikelvin microwave transport measurements, we uncovered the nucleation and thin film microstructure of alpha, beta, and mixed Ta films. We correlated this with impacts on transition temperature and Q-factor.

8:30am **QS-TuM-3 Quantum Engineering of Superconducting Qubits***,* ***William D. Oliver****,* MIT **INVITED**

Superconducting qubits are coherent artificial atoms assembled from electrical circuit elements and microwave optical components. Their lithographic scalability, compatibility with microwave control, and operability at nanosecond time scales all converge to make the superconducting qubit a highly attractive candidate for the constituent logical elements of a quantum information processor.Over the past decade, spectacular improvements in the manufacturing and control of these devices have moved the superconducting qubit modality from the realm of scientific curiosity to the threshold of technical reality. In this talk, we present recent progress, challenges, and opportunities ahead in the engineering of larger scale processors based on superconducting qubits.

9:15am **QS-TuM-6 Characterization of Hydroxyls in Surface Oxides of Tantalum and Their Mitigation for Superconducting Qubits***, **Ekta Bhatia**, N. Pieniazek, A. Biedron, S. Schujman,* NY CREATES*; H. Frost,* Tokyo Electron Ltd. Technology Center America (TTCA) LLC*; Z. Xiao, S. Olson, J. Nalaskowski, K. Musick, T. Murray, C. Johnson, S. Papa Rao,* NY CREATES

Recently, Ta has attracted more attention [1] in the superconducting quantum community due to the high coherence times in superconducting qubits when it replaces Nb in the capacitor pads [2]. The surface oxides of superconducting metals have been demonstrated to be a major contributor to microwave loss mechanisms [3], and hence to decoherence in superconducting qubits. In this study, we quantify the concentration of hydroxyls [OH], and their variation with depth in various surface oxides of Ta. We also demonstrate, for the first time, that it is possible to modulate the extent to which such tantalum hydroxyls are present by replacing the native oxide of Ta with a chemically-formed surface oxide. Using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) analysis, we were able to quantitatively determine the concentrations of TaOH as a function of depth, for both the native oxide of Ta, as well as for the surface oxide that is formed during chemical mechanical planarization of Ta. The effect of fiber texture in the deposited Ta film on the oxidation and the incorporation of [TaOH] was also studied. Angle-resolved X-ray photoelectron spectroscopy was used to study the composition of the surface oxide – specifically, the prevalence of Ta2O5 on the surface, with suboxides of Ta closer to the interface with metallic Ta, with thickness information obtained from transmission electron microscopy. It has been hypothesized [3] that TLS are not uniformly distributed throughout the oxide - our observations not only substantiate that hypothesis but indicate that hydroxyls are a possible molecular origin for such TLS. In a fashion analogous to studies of aluminum oxide [4], where the rotational freedom of the [OH] bond is suggested to be a source of the TLS, it is possible that [OH] plays a similar role in tantalum oxides as well. We also explore ways to modulate TaOH using nitridization on the Ta surface. Our findings provide ways to mitigate the effects of two-level systems in superconducting quantum devices.

[1] S. Papa Rao *et al.*, *Electrochem. Soc. Trans.* **85** (6), 151 (2018).

[2] N.P. de Leon *et al.*, *Science* **372**, eabb2823 (2021).

[3] K. D. Crowley *et al.*, *Phys. Rev. X* **13**, 4 (2023).

[4] L. Gordon *et al., Sci. Rep.* **4**, 7590 (2014).

9:30am **QS-TuM-7 Identifying and Mitigating Sources of Loss in Superconducting Qubits***, **Akshay Murthy**, M. Bal, F. Crisa, S. Zhu, D. Bafia, J. Lee, A. Romanenko, A. Grassellino,* Fermilab **INVITED**

Advances in our understanding of materials has played a crucial role driving recent increases in achievable coherence times and gate fidelities in superconducting transmon qubits. This includes identifying defects, impurities, interfaces, and surfaces present within the device geometry as well as implementing new strategies to mitigate the deleterious effects introduced by these disordered regions. As part of the Superconducting Quantum Materials and Systems (SQMS) center, we have deployed a wide variety of unique materials characterization techniques in tandem with microwave measurements to examine sources of loss in these devices. These include materials characterization techniques such as scanning/transmission electron microscopy, x-ray diffraction/reflectivity, scanning probe microscopy, secondary ion mass spectrometry, and atom probe tomography performed at both room temperature and cryogenic temperatures in addition to microwave loss measurements leveraging high quality factor superconducting radiofrequency (SRF) cavities. Through this effort, researchers have identified a wide variety of defective structures that serve as sources of two-level systems (TLS) or non-TLS dissipation as well as estimate their relative impacts to build a hierarchy of losses.

In this talk, I will discuss our results demonstrating that the surface oxide associated with superconducting niobium metal serves as a major source of microwave loss and that this loss scales with oxygen vacancies present in this oxide region. Based on this insight, we encapsulate the surface of niobium with various metal and dielectric layers that eliminate and prevent the formation of this lossy niobium surface oxide upon exposure to air and systematically achieve coherence times on the order of hundreds of microseconds. In order to continue to extend coherence times such that they reproducibly exceed beyond a millisecond, the loss hierarchy we have developed indicates that additional materials development to eliminate loss associated with the underlying substrate as well as the Josephson junction is needed. During the second half of my talk, I will discuss ongoing efforts in this area as well as the progression along our Quantum Technology roadmap that will move us from individual qubits to scalable, high coherence, multi-qubit platforms.

11:00am **QS-TuM-13 Dielectric Loss and Two-Level Systems in Superconducting Qubits***, **Chen Wang**,* University of Massachusetts **INVITED**

Superconducting circuits are one of the leading technology platforms for the development of a practical quantum computer.In superconducting quantum circuits, qubits are typically constructed from Al/AlOx/Al Josephson tunnel junctions and patterned superconducting thin films such as Al, Nb, Ta on crystalline Si or sapphire substrate, and operated with external microwave pulses.Superconducting qubits enjoy advantages in their circuit design flexibilities, lithographic scalability, and operational clock speed, but must overcome decoherence and parameter variability and fluctuations from the solid-state environment.In particular, microwave noise from dielectric materials, including the Josephson junction, the bulk substrate, and various interfaces, have increasingly stood out as a limiting factor for both the lifetime and frequency stability of superconducting qubits.Such dielectric dissipation and fluctuation have been attributed to the omni-presence of a large number of discrete microscopic two-level systems (TLS) over an extremely broad frequency ranges (from kHz to GHz).Various improvements in qubit design and materials processing have led to substantial improvement of qubit coherence over the past decade through the mitigation of the TLS problem, but any atomistic understanding of these TLS in relevant materials remains elusive.In this talk, I will give a birds-eye view of the phenomenological studies of dielectric loss and two-level systems in superconducting circuits, and explain how the dream of building a quantum computer has been intertwined with so-far the most

sensitive probe and the most demanding quest of traditional but pristine materials.

11:30am **QS-TuM-15 Measuring Loss Tangents of Substrates for Superconducting Qubits with Part per Billion Precision**, ***Daniel Bafia***, *A. Murthy, A. Lunin, G. Nahal, A. Clairmont, M. Bal, A. Romanenko, A. Grassellino,* Fermi National Accelerator Laboratory

This talk will present a comparative study on the dielectric loss tangent of various substrates measured with an ultra-high quality factor niobium SRF cavity at the low electric fields and mK temperatures relevant for superconducting quantum computing architectures. We study the loss tangent evolution of c-plane sapphire post various treatments and correlate the resulting performance with materials analysis including time-of-flight secondary ion mass spectrometry and atomic force microscopy and report on key findings.

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.

11:45am **QS-TuM-16 Enhanced Qubit Frequency Targeting and Quantum Gate Fidelities in a 25-Qubit Superconducting Quantum Processor**, ***Amr Osman***, *L. Chen, H. Li, A. Nylander, M. Rommel, S. Hill, E. Moschandreou, D. Shiri, M. Faucci Giannelli, A. Fadavi Roudsari, G. Tancredi, J. Bylander,* Chalmers University of Technology, Gothenburg, Sweden **INVITED**

Crosstalk poses a significant challenge to the scalability of superconducting quantum processors. This issue can be mitigated by implementing a careful frequency crowding scheme that ensures sufficient separation between neighboring quantum gate frequencies. Nevertheless, deviations in the fabrication process from the design parameters can undermine this scheme, leading to reduced qubit-gate fidelities. In this study, we designed and fabricated a 25-qubit quantum processor in a flip-chip geometry using a specially tailored frequency allocation scheme for parametric-gate architectures [1]. We present an extensive characterization of parameter targeting in this quantum processor, exploring the uncertainties introduced by the flip-chip bonding, and discussing the implications for crosstalk and quantum-gate fidelities.

[1] A. Osman, J. Fernandez-Pendas, C. Warren, S. Kosen, M. Scigliuzzo, A. Frisk Kockum, G. Tancredi, A. Fadavi Roudsari, and J. Bylander, “Mitigation of frequency collisions in superconducting quantum processors,” Phys. Rev. Res. 5, 043001 (2023).

Electronic Materials and Photonics
Room 114 - Session EM+2D+BI+QS+TF-TuA

Advances in Photonic Materials and Devices

Moderators: Leland Nordin, University of Central Florida, **Philip Lee**, University of Kentucky

2:15pm **EM+2D+BI+QS+TF-TuA-1 New Materials for Metamaterials: Electrochemical Materials and Switchable Chiral Nanostructures**, ***Vivian Ferry***, University of Minnesota **INVITED**

Alternative materials for metasurfaces enable new properties and lay the foundation for advantage applications. This talk will discuss two strategies for new, tunable metasurfaces. The first part of the talk will discuss the use of electrolyte gating to control the optical properties of materials, focusing on $La_{1-x}Sr_xCoO_{3-d}$ (LSCO) as an exemplary case. We fabricate electric double layer transistors using LSCO and an ion gel, and under application of positive gate voltage gating facilitates the formation and migration of oxygen vacancies, and a transition from a perovskite phase to an oxygen-vacancy-ordered brownmillerite phase. This is accompanied by substantial change in optical properties, as measured with spectroscopic ellipsometry. The talk will discuss how LSCO can be incorporated with metasurfaces to produce tunable optical response. The second part of the talk will discuss chiral metamaterials, and particularly novel materials comprised of nanopatterned, light emitting nanocrystals with simultaneous control over both directionality and polarization state.

2:45pm **EM+2D+BI+QS+TF-TuA-3 Optoelectronic Nanowire Neuron**, ***Thomas Kjellberg Jensen***, Lund University, Sweden; *J. E. Sestoft,* Niels Bohr Institute, Denmark; *D. Alcer, N. Löfström, V. Flodgren, A. Das,* Lund University, Sweden; *R. D. Schlosser, T. Kanne Nordqvist,* Niels Bohr Institute, Denmark; *M. Borgström,* Lund University, Sweden; *J. Nygård,* Niels Bohr Institute, Denmark; *A. Mikkelsen,* Lund University, Sweden

Three different semiconductor nanowires are combined into a single optoelectronic artificial neuron. In general, artificial neurons sum and weight input signals, and output a signal according to a non-linear function which may be sigmoid-shaped (a generalized artificial neuron is shown in Fig. 1a). Figure 1b schematically shows the artificial neuron realized using nanowires. Here, neural excitation/inhibition is achieved by balancing inputted light across two pin-diode nanowires outputting a summed voltage measured by a nanowire-based field-effect transistor (FET).

The false-colored electron microscope image shown in Figure 1c depicts the fabricated nanowire neuron. In Figure 1d we show the current measured across the FET nanowire as a function of laser beam position, demonstrating the excitatory and inhibitory behavior. Selectively illuminating the excitatory nanowire diode, the change in conductance follows a sigmoidal curve as a function of linearly increasing light intensity (Figure 1e) – the necessary non-linear part of a neural network. Taken together, these properties provide the device with the basic functionalities needed for a neuromorphic computing node [1,2]. Future measurements will explore the time-domain effects.

Our artificial neuron provides a promising future platform for combining diverse materials with low power consumption and significantly reduced circuit footprint, this way addressing critical limitations for future-proofing photonics-based applications in neuromorphic computing.

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[2] D. Winge, M. Borgström, E. Lind, and A. Mikkelsen, "Artificial nanophotonic neuron with internal memory for biologically inspired and reservoir network computing", *Neuromorph. Comput. Eng.*, vol. 3, no. 034011, 2023.

3:00pm **EM+2D+BI+QS+TF-TuA-4 Modulation of Optical and Plasmonic Properties of Epitaxial and Precision Titanium Nitride Thin Films**, *I. Chris-Okoro,* North Carolina A&T State University; *S. Cherono,* North Carolina A & T State Uni; *C. Martin,* Ramapo College of New Jersey; *V. Craciun,* National Institute for Laser, Plasma, and Radiation Physics, Romania; *S. Kim, J. Mahl, J. Yano,* Lawrence Berkeley National Laboratory; *E. Crumlin,* Lawrence Berkeley Lab; ***Dhananjay Kumar***, North Carolina A & T State Uni

The present study arises from the need for developing negative-permittivity materials beyond commonly employed plasmonic metals (e.g., Au, Ag), which are often incompatible (i.e., low melting point, mechanically soft, chemically unstable) with real operating environments. This work reports a pulsed laser-assisted synthesis, detailed structural characterization using x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), x-ray absorption spectroscopy (XAS), Rutherford Backscattering spectroscopy (RBS), and plasmonic properties of three sets of TiN/TiON thin films. The first two sets of TiN films were grown at 600 and 700 °C under a high vacuum condition (≤2 ×10^{-7} Torr). The third set of TiN film was grown in the presence of 5 mTorr of molecular oxygen at 700 °C. The purpose of making these three sets of TiN/TiON films was to understand the role of film crystallinity and the role of the oxygen content of TiN films on their optical and plasmonic properties. The results have shown that TiN films deposited in a high vacuum are metallic, have large reflectance, and high optical conductivity. The TiN films, grown in 5 mTorr, were found to be partially oxidized with room temperature resistivity nearly three times larger than those of the TiN films grown under high vacuum conditions.

The optical conductivity of these films was analyzed using a Kramers-Kronig transformation of reflectance and a Lorentz-Drude model; the optical conductivity determined by two different methods agrees very well. The good agreement between the two methods is indicative of a reliable estimate of the absolute value of reflectance in the first place. The existence of significant spectral weight below the interband absorptions is shared between two Lorentzians, one around 250 cm^{-1} and one around 2,500 cm^{-1}. We discuss here the dependence of the two bands on the deposition conditions and their effect on the plasmonic performances of TiN/TiON thin films, in particular on the surface plasmon polariton (SPP) and localized surface plasmon resonance (LSPR) quality factors.

This work was supported by the NSF PREM on the Collaborative Research and Education in Energy Materials (CREEM) via grant # DMR-2122067 and the DOE EFRC on the Center for Electrochemical Dynamics And Reactions on Surfaces (CEDARS) via grant # DE-SC0023415.

3:15pm **EM+2D+BI+QS+TF-TuA-5 Nano-Focusing and Characterization of the OAM Beam Through an Optical Fiber Using Plasmonic Nanostructure**, ***Rohil Kayastha***, *W. Zhang, B. Birmingham,* Baylor University; *Z. Gao,* Texas A&M University; *J. Hu,* Baylor University; *R. Quintero-Torres,* UNAM, Mexico; *A. V. Sokolov,* Texas A&M University; *Z. Zhang,* Baylor University

Optical vortex beam has been used in many applications such as nanoscale imaging, telecommunication, sensing, and so on due to its unique azimuthal phase distribution. Many of these applications utilize optical fibers as a sensor or to propagate the beam to transmit data and information. The vortex beam carrying an orbital angular momentum (OAM) has a phase singularity giving the beam a doughnut intensity profile. Due to its helical wavefront nature, the vortex beam carrying OAM has also been used to distinguish the enantiomers of the chiral molecule. However, coupling efficiency remains a problem due to the size mismatch of the beam and the molecule. Our work uses vortex fibers with plasmonic nanostructures to nano-focus the vortex beam to enhance the coupling between light and chiral matter. To achieve this goal, characterization of vortex beam in free space and through vortex fiber (a polarization-maintaining ring core optical fiber), and fabrication of nanostructure on fiber facet were performed.

Generation and propagation of OAM beams were characterized in free space and through a vortex fiber. The free-space OAM beam was coupled and transmitted successfully through the vortex fiber with a pure and stable output beam. The helicity characterization and polarization analysis of the free-space and fiber-coupled output vortex beams showed consistent polarization and OAM. The direction of the phase front was maintained after propagation of the OAM through the vortex fiber, as observed from the spiral interference pattern. Nano-focusing of the OAM beam using nanostructure on the fiber facet was observed from the simulation. The circular array of plasmonic nanobars was fabricated on the fiber facet core, and the far-field image of the output OAM beam was observed after transmission through the fiber with the nanostructure. The near-field image of the nano-focused OAM beam on the fiber will be investigated using a near-field scanning optical microscope (NSOM). The focusing of the OAM beam on a fiber facet with the nanostructure could enhance the coupling efficiency of the beam with chiral molecules. The nano-focused OAM on the fiber could be used as a scanning and sensing probe for single-molecule chirality detection.

4:00pm **EM+2D+BI+QS+TF-TuA-8 Templated Block Copolymer Network Thin Films as 3D Chiral Optical Metamaterials: Connecting Finite-Difference Time-Domain and Self-Consistent Field Theory Simulations**, ***Emily McGuinness**, B. Magruder, P. Chen, K. Dorfman, C. Ellison, V. Ferry,* University of Minnesota

Optical metamaterials, whose properties depend not only on material selection but also the spatial arrangement of the material, provide access to interactions with light that are not present in bulk materials alone. Block copolymer self-assembly is a scalable method for creating 3D spatially periodic nanoscale structures to act as metamaterial templates. The gyroid morphology, whose curved, percolating structure is composed of triply connected struts, possesses chiral elements such as helices in bulk and chiral structures at certain surface terminations. As a result of their chirality, when templated with a plasmonic material, gyroids exhibit circular dichroism (CD) with applications in anti-counterfeit as well as molecular and protein sensing. While many optical simulations of gyroids assume a perfect cubic structure, most applications utilize thin films whose processing results in distortions such as compression normal to the substrate or surface rearrangements due to interactions with interfaces. Distorted gyroids, as well as the growing library of additional network structures possible from block copolymer self-assembly, are increasingly challenging to model from a purely mathematical basis and require better basis in physical reality. Combining the output of polymer self-consistent field theory (SCFT) with finite-difference time-domain (FDTD) optical simulations enables the exploration of thermodynamically equilibrated structures for both distorted gyroids and expanded network geometries. This presentation will investigate the CD response of compressed double gyroid thin films as well as that of newly hypothesized network structures such as H^{181}. In the first example, compression of (110) oriented silver double gyroid thin films yields a switching phenomenon from left to right circularly polarized light preferential absorption, offering the potential for dynamic systems (**Figure 1a**). Mechanistically, this behavior depends both on the surface and sub-surface structures of the compressed double gyroids. In the second example, (001) oriented silver templated thin films of the newly computationally uncovered H^{181} structure are shown to support a broadband visible light CD response (spanning 200 nm) with a g-factor (CD normalized to average absorption) of at least 0.14 across that entire wavelength range (**Figure 1b**). Overall, this work moves the optical simulations of metamaterials from block copolymers closer those physically realized, introducing additional opportunities for engineering their optical response.

4:15pm **EM+2D+BI+QS+TF-TuA-9 Solution Processing of Optical Phase Change Materials**, ***Brian Mills,*** Massachusetts Institute of Technology*; R. Sharma, D. Wiedeman,* University of Central Florida*; C. Schwarz,* Ursinus College*; N. Li,* Massachusetts Institute of Technology*; E. Bissell,* University of Central Florida*; C. Constantin Popescu,* massachusetts Institute of Technology*; D. Callahan,* Charles Stark Draper Laboratory, Inc.*; P. Banerjee, K. Richardson,* University of Central Florida*; J. Hu,* Massachusetts Institute of Technology

Chalcogenide optical phase change materials (O-PCM) serve as the functional material in a variety of non-volatile photonic devices, from reconfigurable metasurface lenses to tunable integrated photonic resonators. Although a handful of high figure of merit O-PCMs have been identified and implemented in prototype devices, the space of O-PCM composition remains relatively unexplored, precluding the possibility of application specific choices in material composition that optimize device performance. This is due, in large part, to the lack of time and cost efficient methods for O-PCM thin film deposition and characterization, for which vacuum chamber deposition is the most common method. In this work, we present the first implementation of a solution processing approach for O-PCM film synthesis and deposition, providing evidence of the method's viability in creating high quality, functioning O-PCM films with close adherence to target stoichiometry. This method serves as a robust platform for materials exploration of O-PCM composition and allows for the identification of candidate O-PCM, as well as an understanding of the effect of compositional changes in O-PCM optical and cycling properties.

4:30pm **EM+2D+BI+QS+TF-TuA-10 Effects of Ce Concentration on the Microstructural, Optical, and Luminescence Properties in Ce:GAGG Ceramic Phosphors**, ***William Bowman**, S. Lass,* University of Central Florida*; F. Moretti, W. Wolszczak,* Lawrence Berkeley National Laboratory*; R. Gaume,* University of Central Florida

Efficient luminescence and optical quality are necessary phosphor attributes for applications such as down-conversion layers in photovoltaics and computed tomography. Cerium-doped gadolinium aluminum gallium garnet (Ce:GAGG) is highly applicable for these purposes. It has been shown in other garnet hosts such as Ce:YAG and Ce:LuAG that Ce concentration alters both the luminescence and optical properties of the materials. In the case of Ce:GAGG single crystals and Ce concentrations lower than 1 at%, radioluminescence decay constants decrease by increasing the Ce concentration while light yield reaches a maximum at 0.3 at%. For Ce:GAGG ceramics, the effect of Ce concentration on these properties has not been systematically investigated. There is at current no work on determining the solid solubility limit of Ce in GAGG, which is critical in controlling the development of secondary phases and subsequent optical quality.

This study aims to investigate the effects of Ce concentration on the microstructural, optical, and luminescence properties of GAGG optical ceramics with dopant concentrations in the 0.1at% to 10at% range. Transmission of the material increases with increasing Ce concentration up to 5.0at%. At the same time, the optical and luminescence properties of these samples show a complex evolution upon Ce concentration, highlighting the complex interplay among optical characteristics of the samples, concentration-related luminescence quenching phenomena, and charge carrier trapping defects.

This material is based upon work supported by the U.S. Department of Homeland Security under Grant Award Number 20CWDARI00038-01-00. The views and conclusions contained in this document are those of the authors and should not be interpreted as necessarily representing the official policies, either expressed or implied, of the U.S. Department of Homeland Security.

4:45pm **EM+2D+BI+QS+TF-TuA-11 Solution Based Processing of $Ge_2Sb_2Se_4Te_1$ Phase Change Material for Optical Applications**, ***Daniel Wiedeman**, R. Sharma, E. Bissel, P. Banerjee,* University of Central Florida*; B. Mills, J. Hu,* Massachusetts Institute of Technology*; M. Sykes, J. Stackawitz, J. Lucinec, C. Schwarz,* Ursinus College*; K. Richardson,* University of Central Florida

Chalcogenide based phase change materials are important for creating novel optical and photonic devices, improving on current devices for future applications. Solution processing, via dip coating, spin coating, or drop-casting, is a low-cost, high-throughput alternative method of depositing thin films, which allows for greater composition diversity. In this work, we performed a detailed systematic study of the solution derived drop-casted film of Ge2Sb2Se4Te1 alloy in an ethylenediamine and ethanedithiol mixture. The composition, morphology and structural properties of the films were analyzed by employing scanning electron microscopy, energy dispersive X-ray spectroscopy, Raman spectroscopy, and X-ray diffraction. Our findings provide insight into a potential route for scalable $Ge_2Sb_2Se_4Te_1$ films.

5:00pm **EM+2D+BI+QS+TF-TuA-12 Multi-Dimensional p-WSe_2/n-Ga_2O_3 Enhancement-Mode Phototransistors for Stand-Alone Deep-Ultraviolet Sensing**, *J. Kim,* ***Soobeen Lee**,* Seoul National University, South Korea

β-Ga_2O_3 is an ultra-wide bandgap (UWBG) semiconductor with a bandgap of 4.9 eV, resulting in a high breakdown field of approximately 8 MV/cm and a high Baliga's figure-of-merit. β-Ga_2O_3 is a promising material for deep-ultraviolet (DUV) photodetector (PD) applications due to its direct bandgap of 4.9 eV, excellent thermal stability, and high absorption coefficient. Self-powered β-Ga_2O_3 PDs can be realized through p-n heterojunction (HJ) field-effect transistor architectures, exhibiting normally-off operation owing to the depletion region in the β-Ga_2O_3 channel. With intrinsic n-type conductivity caused by unintentional doping and challenges in p-type doping, fabricating self-powered β-Ga_2O_3 PDs necessitates combining β-Ga_2O_3 with p-type semiconductors such as transition-metal dichalcogenides (TMDs), nickel oxide, or silicon carbide. Tungsten diselenide (WSe_2), one of the TMDs, stands out as a promising material with a high monolayer mobility of approximately 180 $cm^2V^{-1}s^{-1}$. Their dangling-bond-free surfaces provide an advantage in forming sharp interfaces with other materials in HJs. Moreover, efficient p-type doping of WSe_2 is achieved via charge transfer by utilizing the high electron affinity of its self-limiting oxide, sub-stoichiometric tungsten oxide (WO_{3-x}), which is used as a dopant.

In this work, we introduce normally-off p-WSe_2/n-β-Ga_2O_3 phototransistors and demonstrate their self-powered operation under 254 nm light. p-Type WSe_2 was realized through charge transfer doping of WO_{3-x} formed by O_3 treatment, and the p-type doping effect of this oxide was confirmed through electrical characteristics. The cross-sectional structure of the fabricated p-WSe_2/n-β-Ga_2O_3 phototransistors was analyzed, and the

electrical and optical properties were evaluated before and after WSe_2 oxidation. The device demonstrated a responsivity of 2 A/W under 254 nm light without an external bias, surpassing the performance of previously reported p-n HJ-based β-Ga_2O_3 PDs. Furthermore, we investigate the enhanced optoelectronic performance of multi-dimensional β-Ga_2O_3 phototransistors with plasmonic metal nanoparticles. In this presentation, we will discuss the potential of the self-powered multi-dimensional DUV β-Ga_2O_3 PDs with improved performance and their prospects in practical applications.

This work was supported by Korea Institute for Advancement of Technology (KIAT) grant funded by the Korea Government (P0012451, The Competency Development Program for Industry Specialist) and the Korea Research Institute for defense Technology planning and advancement (KRIT) grant funded by Defense Acquisition Program Administration (DAPA) (KRIT-CT-21-034, and KRIT-CT-22-046).

Quantum Science and Technology Mini-Symposium
Room 123 - Session QS-TuA

Advances in Quantum Dots and Dynamic Effects in Josephson Junctions

Moderators: Sisira Kanhirathingal, Rigetti Computing, **Ekta Bhatia**, NY CREATES

2:15pm **QS-TuA-1 Toward Robust Spin-Optical Interfaces in Molecular Spin Qubits**, ***Leah Weiss***, *G. Smith,* University of Chicago*; R. Murphy, B. Golesorkhi, J. Long,* University of California at Berkeley*; D. Awschalom,* University of Chicago **INVITED**

Efficient spin-optical interfaces play a key role in quantum technologies ranging from generation of multi-qubit entangled states to remote nanoscale quantum sensing. This interface can be designed from the bottom up in organometallic molecules to enable optical initialization and read out of ground-state molecular spins [1], providing a synthetic analog of solid-state spin qubits. We have shown that by changing the atomic structure of either the molecule or its local environment, the spin and optical properties of this class of qubits can be chemically modified [2,3]. Building on these demonstrations, we report the development of molecular ground-state spin qubits with robust spin-optical coupling. We utilize the observed spin-photon interface to demonstrate all-optical detection of ground-state spin properties in molecular ensembles. These results open avenues for the tailored design of molecular qubits for targeted sensing applications requiring efficient coupling of spins with photons.

[1] S. L. Bayliss,et al., Science. **370**, 6522 (2020).

[2] D. W. Laorenza, et al. JACS. **143**, 50 (2021).

[3] S. L. Bayliss, et al. Phys. Rev. X. **12,** 3 (2022).

2:45pm **QS-TuA-3 Development of a Flip-Chip Induced Quantum Dot Device with Semiconductor Materials**, ***Giovanni Franco-Rivera***, *J. Marbey, M. Dryer, R. Butera,* Laboratory for Physical Sciences

The ability of the semiconducting industry to manufacture advanced technology devices is expected to speed up the development of quantum computing. Confining few electrons in silicon-based heterostructures via lithographically-designed, gated on-chip quantum dots (QD) enables the manipulation of the spin degree of freedom for quantum information processing. Some of the appealing features of the QD spin qubits are their long coherent properties [1] achievable by solid-state all-electrical control readout [2] leading to recent demonstrations of high fidelity multiqubit operations [3]. However, performance of current state-of-the art QD qubits is typically limited by the fundamental properties of the underlying materials. Moreover, the exploration of new quantum materials as potential hosts of spin qubits is often overlooked due to the complications resulting from developing an overwhelming fabrication process. We propose an alternative method based on a flip-chip geometry allowing a QD to be induced on an arbitrary material of interest. The control chip, separated from the host material by ~100nm, contains all the necessary circuit elements for gating and readout of the QD structure. A vacuum gap separates the control and host chips via an engineered mesa recess and bonding pads. We will present the efforts on the integrated flip-chip design based on a control silicon chip and a host Ge/SiGe heterostructure target chip. Lastly, fabrication efforts and device screening measurements for on-chip Ge/SiGe QD structures are presented enabling future comparison of the device performance between on-chip and flip-chip architectures.[1] J. T. Muhonen et al., Nature Nanotech. 9, 986-991 (2014).[2] P. Harvey-Collard et al., Phys. Rev. X 8, 021046 (2018).[3] A. R. Mills et al., Sci. Adv.8, eabn5130 (2022).

3:00pm **QS-TuA-4 Nanoscale Spatial Control of Colloidal Quantum Dots and Rods Using DNA for Next-Generation Quantum Devices**, *X. Luo, C. Chen,* ***Mark Bathe***, MIT

Advances in photonic quantum technologies require precise control over quantum emitters at sub-10 nanometer scales for quantum computing and sensing applications. Conventional top-down fabrication methods face limitations in resolution and scalability on this front. In contrast, scalable bottom-up approaches utilizing DNA self-assembly offer unprecedented control over colloidal quantum materials at the nanoscale, such as quantum dots (QDs) and rods (QRs). We program and manipulate QDs and QRs using DNA nanostructures as templates, towards their scalable and precise incorporation into quantum photonic devices. DNA nanotechnology has emerged with unparalleled versatility and accuracy in creating complex, programmable architectures at the nano- to micro- scale (1, 2). Using versatile 3D wireframe DNA templates of customized geometry and chimeric single-stranded DNA (ssDNA) wrapping, we developed a general strategy to program ssDNA valences on QD surfaces (3). This valence-geocoding approach enabled the fabrication of QD energy transfer circuits (3). Using a rigid, planar wireframe DNA origami template, we arranged aligned QRs into 2D arrays on surfaces with nanoscale precision (4). We developed an ultrafast dehydration-assisted method to conjugate a dense layer of ssDNA onto QDs/QRs directly from organic solvent to facilitate their precise and stable assembly to 2D DNA template lattices up to a micron in size (4). To integrate DNA templated QDs/QRs into chip-based photonic devices, we further employed electron beam lithography (EBL) to guide the deterministic patterning of precisely positioned and oriented DNA templates on silicon chips, which were then used to template QDs and QRs with nanoscale accuracy. Scalable production of DNA templates using biologically produced DNA molecules (5) and its application in quantum photonics aligns with initiatives promoting biomanufacturing innovation for a sustainable bioeconomy (6). Combining the strengths of top-down lithography methods and bottom-up DNA self-assembly holds the potential of a scalable, parallel and environmentally benign nanofabrication framework that accurately patterns single colloidal quantum emitters over 2D surfaces on the wafer-scale.

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2. Knappe, G.A., et al. (2023). Nature Reviews Materials, 8: 123.
3. Chen, C., et al., (2022). Nature Communications, 13: 4935.
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3:15pm **QS-TuA-5 Characterization of epitaxially grown Al-Ge/SiGe quantum wells for voltage-controlled Josephson junctions**, ***Joshua Thompson***, Laboratory for Physical Sciences*; S. Davari,* University of Arkansas*; C. Gaspe, K. Sardashti,* Laboratory for Physical Sciences*; H. Churchill,* University of Arkansas*; C. Richardson,* Laboratory for Physical Sciences

Strained germanium quantum wells host heavy holes with high mobility and low effective mass, which combined with highly transparent epitaxial aluminum creates a promising platform for voltage-controlled superconductor-semiconductor devices that are compatible with standard Si fabrication methods. This talk will discuss the characterization of undoped germanium quantum wells in a SiGe heterostructure grown by molecular beam epitaxy and the fabrication of planar Josephson junctions. By applying an electrostatic gate, the induced two-dimensional hole gas was observed to have a carrier mobility > $2x10^4$ cm^2/Vs with a density < $1x10^{12}$ cm^{-2}. Using an etch process, 50-100 nm Josephson junctions where fabricated on a tall mesa structure and characterized by measuring I_CR_N and the supercurrent dependance on applied gated voltage and magnetic field.

4:00pm **QS-TuA-8 Developing a Novel Approach to Extract the Current-Phase Relation of Josephson Junctions with On-Wafer Microwave Probing and Calibration Techniques**, ***Elyse McEntee Wei***, Colorado School of Mines*; P. Dresselhaus, A. Fox, D. Williams, C. Long,* National Institute of Standards and Technology, Boulder*; S. Eley,* University of Washington

We are developing a novel approach to characterize the current-phase relation (CPR) of Josephson junctions using on-wafer microwave probing and calibration techniques. Josephson junctions are the integral component in superconducting quantum circuits and exhibit a supercurrent that is modulated by a function of the phase difference between the order parameters of the superconducting electrodes, known as the CPR. Typically, the CPR is assumed to be sinusoidal. However, skewing has been observed in junctions with various barrier compositions such as normal metals,

ferromagnetic materials, InAs nanowires, and graphene. This skewing can significantly affect the output of devices such as timing in single-flux quantum circuits used for digital logic, as well as the harmonic power in pulsed junction arrays used in voltage standards. The CPR is commonly measured using specialized superconducting quantum interference device (SQUID) circuitry. However SQUIDs are very sensitive to flux noise and can easily couple to nearby circuit components, limiting the ability of the SQUID circuit to measure the CPR. Our approach employs a homebuilt cryogenic probe station for measurements of Josephson junction arrays embedded in superconducting coplanar waveguides. It then involves extracting the Josephson inductance from Josephson transmission lines as a function of bias current using scattering-parameters calibrated with an on-wafer multiline Thru-Reflect-Line calibration to reconstruct the CPR. Here, we apply this approach to studying the CPR in niobium-doped amorphous silicon Josephson junction arrays, in which preliminary data shows evidence of skewing and higher order harmonics. Upon validation, this novel approach would offer broadband, low noise measurements of the CPR, providing critical design information for circuits that are based on Josephson junctions.

4:15pm **QS-TuA-9 Aging effects after Alternating Bias Assisted Annealing of Josephson Junctions**, ***David P. Pappas***, *X. Wang, J. Howard, E. Sete,* Rigetti Computing*; G. Stiehl,* rice University*; S. Poletto, X. Wu, M. Field, N. Sharac, C. Eckberg, H. Cansizoglu, J. Mutus, K. Yadavalli, A. Bestwick,* Rigetti Computing

New avenues of trimming the resistance of Josephson junctions promise to allow for precise frequency allocation. This can be expected to significantly improve the yield and fidelity of chips and measurements, respectively. In this talk we will discuss the stability of the junction normal resistance over a wide range of time scales.

4:30pm **QS-TuA-10 Evaluating Radiation Impact on Transmon Qubits Using a Fast Decay Protocol in Above and Underground Laboratories**, ***Tanay Roy***, Fermi Lab

Superconducting qubits can be sensitive to sudden energy deposits caused by ambient radioactivity and cosmic rays. Previous studies have focused on understanding possible correlated effects over time and distance due to this radiation. In this study, for the first time, we directly compare the response of a transmon qubit measured initially at the SQMS above-ground facility (Fermilab, Illinois, USA) and then at the deep underground Gran Sasso Laboratory (INFN-LNGS, Italy). We observe the same average qubit lifetime of roughly 80 microseconds at both facilities. We then apply a fast decay detection protocol and investigate the time structure and relative rates of triggered events due to radiation versus intrinsic noise, comparing the above and underground performance of several high-coherence qubits. Using gamma sources of variable intensity we calibrate the response of the qubit to different levels of radiation in an environment with minimal background radiation. Results indicate that qubits respond to a strong gamma source, and it is possible to detect particle impacts. However, we do not observe a difference in radiation-induced-like events when comparing the above and underground results for niobium-based transmon qubits with sapphire substrates. We conclude that the majority of these events are not radiation-related and are attributed to other noise sources, which by far dominate single-qubit errors in modern transmon qubits.

[1] Dominicis, Roy et al. arXiv:2405.18355

4:45pm **QS-TuA-11 Quantum Enhanced Josephson Junction Field-Effect Transistors for Logic Applications**, ***W. Pan***, *A. Muhowski, W. Martinez, C. Sovinec, J. Mendez, D. Mamaluy,* Sandia National Laboratories

Josephson junction field-effect transistors (JJFET, Fig. 1a) have recently emerged as a promising candidate for low-energy, power-efficient microelectronics applications. JJFETs are particularly useful for low power consumption applications as they are operated with, in the superconducting regime, zero voltage drop across its source and drain. For JJFETs to perform logic operations, the gain-factor (a_R) value must be larger than 1. Here $a_R = dIc/d(Vg–Vt) \times \pi\Delta/Ic$, Δ is the superconducting gap, Vg the gate bias voltage, Vt the threshold voltage. $Ic \sim \exp(-L/\xi_c)$ is the critical supercurrent, where L is the channel length and ξ_c the carrier coherence length. In a conventional JJFET, $\xi c \sim (Vg–Vt)0.5$ (Fig. 1b), and thus $dIc/d(Vg–Vt)$ is small (Fig. 1c). This translates to a requirement of superconducting transition temperature of ~ 400K for a_R larger than 1, far exceeding any recorded critical temperatures. As such, it is impossible to use conventional JJFETs for logic operations. Here, we propose a novel type of JJFET based on quantum phase transition, such as the excitonic insulator (EI) transition in an InAs/GaSb type-II heterostructure, for low-energy, power-efficient logic applications. The nature of the collective phenomenon in the EI quantum phase transition can provide a sharp transition of the supercurrent states (e.g., $\xi_c \sim (Vg–Vt)5$ and $dIc/d(Vg–Vt)$ very large, as shown in Figs. 1b and 1c, respectively) which will enable a_R larger than 1 with an easy-to-achieve superconducting transition temperature, e.g., ~ 40K.

In this talk, we will present some preliminary results demonstrating that indeed the gain factor in these quantum enhanced JJFETs can be greatly improved, thus making them a promising candidate for logic applications. Fig. 2a shows a JJFET made of a zero-gap InAs/GaSb heterostructure with tantalum (Ta) as the source and drain electrodes. The superconducting critical current in the JJFET is zero when $Vg\text{-}Vt \leq 0.23V$, but sharply jumps to a finite value at $Vg\text{-}Vt = 0.24V$ and then increases slowly as Vg-Vt continues to increase (Fig. 2b). The gain factor is calculated to be ~ 0.06. Though still less than 1, it is already more than 50 times larger than that recently reported in a conventional JJFET made of InAs quantum wells. With further optimization, a sharper excitonic insulator transition can be achieved. Together with a higher superconducting transition temperature, a large gain factor can be expected.

5:00pm **QS-TuA-12 Revealing Signatures of Unconventional Superconductivity in Tunneling Andreev Spectroscopy**, ***Petro Maksymovych***, *S. Song,* Oak Ridge National Laboratory*; C. Lane,* Los Alamos National Laboratory*; J. Wang,* Oak Ridge National Laboratory*; W. Ko,* University of Tennessee Knoxville*; J. Lado,* Aalto University, Finland

Understanding order parameter symmetry in superconductors continues to be a frontier topic in condensed matter, particularly with the recent surge of new superconducting materials and their prospective applications in quantum information processing. Recently we introduced a new technique to detect Andreev reflection across the tunneling gap - dubbed Tunneling Andreev Reflection (TAR) [1] - which essentially measures the probability of injecting Cooper pairs with atomic-scale contacts. When combined with scanning tunneling microscopy (STM), this method can achieve true atomic-scale imaging of the superconducting state and extend the ability of STM to probe pairing symmetry, magnetism, and topological properties by analogy with Andreev measurements in devices and heterostructures. For example, we used TAR to unambiguously confirm the sign-changing order parameter in paradigmatic FeSe, and further revealed suppression of superconductivity along the nematic twin boundaries above 1.2 K [2].

To achieve atomic-scale resolution, TAR makes a necessary trade-off in the loss of momentum resolution. It is one of the main differences between TAR and the more traditional, point contact method to measure Andreev reflection, and one the requires a fundamental rethinking of the origins of specific tunneling Andreev spectra. In this talk, based on detailed tight-binding modeling of model Hamiltonians with support from model experiments, we will reveal the basic mechanisms by which TAR spectra connect to the properties of the superconductor. Remarkably, the key ingredients of these spectra can all be rationalized by considering four contributing phenomena: (1) competition between Andreev and single electron tunneling in any given junction; (2) electronic changes of the conductance spectra as a function of increasing coupling strength; (3) energy-dependence of Andreev tunneling, particularly for sign-changing and nodal order parameters; (4) specific details of the band structure. Therefore, tunneling Andreev spectra will in general reflect both intrinsic properties of the superconductor as well as those of the tunneling transport - providing a wealth of information to characterize complicated materials and dramatically expanding the ability of tunneling spectroscopy to search for exotic quantum materials. Research sponsored by Division of Materials Science and Engineering, Basic Energy Sciences, Office of Science, US DOE. SPM experiments were carried at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, a US DOE User Facility.

2D Materials

Room 122 - Session 2D+EM+MI+QS-WeM

2D Materials: Heterostructures, Twistronics, and Proximity Effects

Moderators: Aaron Bostwick, Advanced Light Source, Lawrence Berkeley National Laboratory, **Tiancong Zhu**, Purdue University

8:00am **2D+EM+MI+QS-WeM-1 Van der Waals Semiconductors: From Stacking-Controlled Crystals to Unconventional Heterostructures**, ***Peter Sutter***, *E. Sutter,* University of Nebraska - Lincoln **INVITED**

2D materials have attracted broad interest due to novel properties that arise in atomically thin crystals. As interesting scientifically and important technologically, but much less explored are van der Waals (vdW) crystals that, assembled from 2D building blocks, lie between a monolayer and the bulk. In this regime, phenomena such as phase separation, transformations between crystal polymorphs, and competition between different stacking registries provide unprecedented opportunities for controlling morphology, interface formation, and novel degrees of freedom such as interlayer twist. But going beyond a single layer also poses significant challenges, both due to the diversity of the possible few-layer structures and the difficulty of probing functionality such as optoelectronics and ferroics at the relevant length scales.

Here, we discuss our recent research that addresses these challenges focusing on group IVA chalcogenides, an emerging class of anisotropic layered semiconductors promising for energy conversion, optoelectronics, and information processing. Advanced *in-situ* microscopy provides insights into the growth process, interlayer twisting,and emerging functionality such as stacking-controlled ferroelectricity. Nanometer-scale electron excited spectroscopy identifies photonic light-matter hybrid states and reveals anisotropic and valley-selective charge carrier flows across interfaces in heterostructures. Our results highlight the rich sets of materials architectures and functionalities that can be realized in van der Waals crystals and heterostructures beyond the 2D limit.

8:30am **2D+EM+MI+QS-WeM-3 Deterministic Assembly, Transfer, and Flipping of 2D Materials Using Tunable Polymer Films**, ***Jeffrey J. Schwartz***, *S. Le,* University of Maryland, College Park*; K. Grutter, A. Hanbicki, A. Friedman,* Laboratory for Physical Sciences

Assembly of two-dimensional (2D) materials into van der Waals heterostructures is a crucial step in creating precisely engineered nanoscale and quantum devices for use in a wide variety of spintronic, electronic, and other applications. Numerous strategies exist to pick-up, stack, transfer, and even flip over these atomically thin structures. One popular strategy leverages the ability to tune the adhesion between a polymer stamp and 2D sheets to pick-up, stack, and release structures at different temperatures. Although relatively easy to implement, this technique is tedious to perform and has a low throughput. Here, we demonstrate a significant improvement to a deterministic, all-dry, polymer-assisted transfer technique using polyvinyl chloride (PVC) thin films to manipulate 2D materials and to fabricate devices. We construct stamps from pairs of commercially available PVC films that controllably pick-up and release 2D sheets within known, overlapping temperature ranges. These mechanically durable stamps can be produced quickly and without the time-consuming preparation and annealing steps required by most other commonly used polymers. Importantly, these stamps not only facilitate deterministic transfer of 2D materials, but they also enable polymer-to-polymer transfer (e.g., between separate stamps) and flipping of material stacks to create inverted heterostructures that are important for many applications, including scanning tunneling microscopy measurements. We characterize the thermal transition properties of the PVC films employed here as well as assay the cleanliness and performance of devices produced using this technique. These improvements enable rapid production of 2D devices with fewer interactions required by the operator, which is especially significant when working in controlled environments (e.g., glovebox) or in remote or autonomously controlled contexts.

8:45am **2D+EM+MI+QS-WeM-4 Cleaning of Low-Dimensionality Materials: Challenge and Solutions**, ***Jean-Francois de Marneffe***, *P. Wyndaele, M. Timmermans, C. Cunha,* IMEC, Belgium*; B. Canto, Z. Wang,* AMO GmbH, Aachen, Germany*; R. Slaets, G. He, I. Asselberghs, C. J. Lockhart de la Rosa, G. Sankar Kar, C. Merckling, S. De Gendt,* IMEC, Belgium

Over the last few years, significant efforts have been made in exploring low-dimensionality materials such as single layer Graphene (SLG), transition metal dichalcogenides (TMDCs) and carbon nanotubes (CNTs), for a wide range of applications covering beyond CMOS logic, EUV pellicles, photonics, and sensing (amongst others). Due to their intrinsic 2D or 1D nature, these materials are highly sensitive to processing damage leading to stoichiometric changes or crystalline defects. Among the many manufacturing steps required for building devices, the cleaning of these systems is an absolute requirement and a bottleneck. Typically, during processing, residual polymers or carbon of ambient origin, do contaminate the surface leading to nanometric deposits that change the intrinsic transport/optical properties of the materials, and cause parasitic dielectric drift or high contact resistance. Wet cleaning, using organic solvents, is a mainstream approach, which proves to be inefficient for irreversibly physically adsorbed polymer residues. In this paper, we explore dry cleaning approaches, based on plasma treatment and UV cure. Plasma-based cleaning proves to be very efficient but leads to material damage, which can be minimized by tuning the average ion energy, the processing temperature, the plasma chemistry or adding a post-cleaning restoration step. For TMDCs, damage consist essentially in the creation of chalcogen vacancies, which lead to metal oxidation upon ambient exposure. For Graphene and CNTs, damage consist in carbon vacancies, causing lattice distortions, oxidation and ultimately a dramatic change of the material's transport properties. Part of this presentation will explore the use of UV cure, which is a known method for cleaning polymers from semiconductor surfaces.

9:00am **2D+EM+MI+QS-WeM-5 Spin-Valley Physics in Mixed-Dimensional Van Der Waals Heterostructures**, ***Vikram Deshpande***, University of Utah **INVITED**

Spin-valley physics has become ubiquitous in 2D materials-based van der Waals (vdW) heterostructures, particularly those hosting flat bands, wherein various ground states with spin-valley character including magnetic, insulating and superconducting states have been observed. On the other hand, mixed dimensional vdW heterostructures, such as those between 2D and 1D materials have been less explored for intricate spin-valley physics. The reduced phase space for scattering in 1D in particular might lead to qualitatively different phenomena. We are guided by our studies of ultraclean carbon nanotube quantum dots wherein we have observed subtle effects from the degeneracy lifting between the speeds of right- and left-moving electrons within a given Dirac cone or valley. Bound states can be purely fast-moving or purely slow-moving, giving rise to incommensurate energy level spacings and a vernier spectrum. Using quantum interferometry [1] and Coulomb blockade spectroscopy [2] of such ultraclean carbon nanotube quantum dots, we have found evidence for this vernier spectrum. The addition-energy spectrum of the quantum dots reveals an energy-level structure that oscillates between aligned and misaligned energy levels. Our data find that the fast- and slow-moving bound states hybridize at certain gate voltages. We extend existing theory to show that our experiment probes the degree of isospin polarization/hybridization of the various quantum states probed in our system. As a result, gate-voltage tuning can select states with varying degrees of hybridization, suggesting numerous applications based on accessing this isospin degree of freedom in conjunction with 2D materials in the form of mixed dimensional vdW heterostructures. We have fabricated prototypical mixed dimensional vdW heterostructures between carbon nanotubes and 2D materials and extended our measurements to these structures. I will discuss our recent and ongoing work studying spin-valley physics in such systems.

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9:30am **2D+EM+MI+QS-WeM-7 Exploring Incommensurate Lattice Modulations in BSCCO van der Waals Heterostructures: Implications for Q-Bit Development**, ***Patryk Wasik***, Brookhaven National Laboratory*; S. Zhao,* Harvard University*; R. Jangid,* Brookhaven National Laboratory*; A. Cui,* Harvard University*; J. Sinsheimer,* Brookhaven National Laboratory*; P. Kim,* Harvard University*; N. Poccia,* IFW Dresden, Germany*; C. Mazzoli,* Brookhaven National Laboratory

Quantum computers (QC) are poised to revolutionise computational capabilities by naturally encoding complex quantum computations, thereby

significantly improving computation time compared to silicon-based technologies. Currently, Q-bits, the essential components of QCs, are made from conventional superconductors that operate efficiently only near absolute zero temperatures. To address this limitation, two-dimensional van der Waals (vdW) encapsulated high-temperature superconductor (HTSC) stacks have been proposed as future Q-bit candidates, driven by recent advancements in nanofabrication techniques. However, a detailed understanding of their structural and electronic properties is crucial.

We present low-temperature resonant soft X-ray investigations on ultrathin $Bi_2Sr_2CaCu_2O_{8+\gamma}$ (BSCCO) vdW heterostructures, promising candidates for large-scale Q-bit applications. BSCCO crystals exhibit two incommensurate lattice modulations (ILMs), providing an excellent opportunity to explore the relationship between structure and electronic behaviour in low dimensions. We report ILMs (Cu L_3) and structural peak (off resonance) maps obtained across the superconducting transition temperature ($T_c \approx 60$ K). These signals, under external gating, present significant potential for further exploration offering new insights into the electronic interactions in vdW HTSC systems.

11:00am **2D+EM+MI+QS-WeM-13 Recent Progresses in van der Waals Layered Magnetic Semiconductors**, ***Young Hee Lee,*** Sungkyunkwan University, Republic of Korea **INVITED**

Ferromagnetism in van der Waals two-dimensional (2D) materials has been reported recently. Intrinsic CrI_3 and $CrGeTe_3$ semiconductors reveal ferromagnetism but the Tc is still low below 60K. In contrast, monolayer VSe_2 is ferromagnetic metal with Tc above room temperature but incapable of controlling its switching via gating due to metallic nature. Moreover, the long-range ferromagnetic order in diluted metal chalcogenide semiconductors has not been demonstrated at room temperature. The key research target is to realize the long-range order ferromagnetism, Tc over room temperature, and semiconductor with gate tunability. In this talk, we introduce magnetic dopant, vanadium in semiconducting WSe_2 and manifest Tc at room temperature and gate tunability at low doping concentration. We further explore different doping concentrations including highly degenerate regime and demonstrate unconventional magnetic order by random telegraph spin noises via interlayer coupling and more recent progresses.

Keywords: Diluted magnetic semiconductor, ferromagnetism, long-range magnetic order, Curie temperature, gate-tunability

Reference

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11:30am **2D+EM+MI+QS-WeM-15 Writing and Detecting Topological Spin Textures in Exfoliated Fe_5-xGete$_2$**, ***Luis Balicas,*** Florida State University - National High Magnetic Field Lab - FSU Quantum Initiative

$Fe_{5-x}GeTe_2$ is a centrosymmetric, layered van der Waals (vdW) ferromagnet that displays Curie temperatures T_c (270-330 K) that are within the useful range for spintronic applications. Little is known about the interplay between its topological spin textures (e.g., merons, skyrmions) with technologically relevant transport properties such as the topological Hall effect (THE), or topological thermal transport. We found via high-resolution Lorentz transmission electron microscopy that merons and anti-meron pairs coexist with Néel skyrmions in $Fe_{5-x}GeTe_2$ over a wide range of temperatures and probe their effects on thermal and electrical transport [1]. It turns out that we detect a THE, even at room T, that senses merons at higher T's as well as their coexistence with skyrmions as T is lowered, indicating an on-demand thermally driven formation of either type of spin texture.Remarkably, we also observe an unconventional THE, i.e., in absence of Lorentz force, and attribute it to the interaction between charge carriers and magnetic field-induced chiral spin textures. We find that both the anomalous Hall effect (AHE) and THE can be amplified considerably by just adjusting the thickness of exfoliated $Fe_{5-x}GeTe_2$, with the THE becoming observable even under zero magnetic field due to a field-induced unbalance in topological charges [2]. Using a complementary suite of techniques, including electronic transport, Lorentz transmission electron microscopy, and micromagnetic simulations, we reveal the emergence of substantial coercive fields upon exfoliation, which are absent in the bulk, implying thickness-dependent magnetic interactions that affect the topological spin textures (TSTs). We detected a 'magic' thickness of t ~30 nm where the formation of TSTs is maximized, inducing large magnitudes for the topological charge density, and the concomitant AHE and THE resistivities at T ~ 120 K. Their values are observed to be higher than those found in magnetic topological insulators and, so far, the largest reported for 2D magnets. The hitherto unobserved THE under zero magnetic field could provide a platform for the writing and electrical detection of TSTs aiming at energy-efficient devices based on vdW ferromagnets.

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Electronic Materials and Photonics
Room 114 - Session EM+AIML+AP+QS+TF-WeM
Ferroelectrics and Memory Devices

Moderators: Samantha Jaszewski, Sandia National Labs, **Erin Cleveland**, Laboratory of Physical Sciences

8:00am **EM+AIML+AP+QS+TF-WeM-1 A Scalable Ferroelectric Non-Volatile Memory Operating at High Temperature**, ***Dhiren Pradhan,*** Department of Electrical and Systems Engineering, University of Pennsylvania*; D. Moore,* 2Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB*; G. Kim,* Department of Engineering Chemistry, Chungbuk National University, Cheongju, Republic of Korea*; Y. He,* Department of Electrical and Systems Engineering, University of Pennsylvania*; P. Musavigharavi,* Department of Materials Science and Engineering, University of Central Florida*; K. Kim, N. Sharma, Z. Han, X. Du,* Department of Electrical and Systems Engineering, University of Pennsylvania*; V. Puli,* Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB*; E. Stach,* Department of Materials Science and Engineering, University of Pennsylvania*; W. Kennedy, N. Glavin,* Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB*; R. Olsson III, D. Jariwala,* Department of Electrical and Systems Engineering, University of Pennsylvania

Non-volatile memory (NVM) devices that reliably operate at temperatures above 300 °C are currently non-existent and remain a critically unmet challenge in the development of high- temperature (T) resilient electronics. There are numerous emerging harsh environment applications including aerospace, space exploration, oil and gas exploration, nuclear plants, mining and others that require complex, in-situ computing and sensing capabilities, for which high temperature NVM is critical. Current Silicon (Si)-based micro(nano)electronics, utilizing complementary metal oxide semiconductor (CMOS) technology, encounter reliability challenges above 200 °C and cannot retain their functional properties at high temperatures. Ferroelectric $Al_xSc_{1-x}N$ exhibits strong potential for utilization in NVM devices operating at very high temperatures (> 500 °C) given its stable and high remnant polarization (P_R) above 100μC/cm^2 with demonstrated ferroelectric transition temperature (T_C) > 1000 °C. Here, we demonstrate an $Al_{0.68}Sc_{0.32}N$ ferroelectric diode based NVM device that can reliably operate with clear ferroelectric switching up to 600 °C with distinguishable On and Off states. The coercive field (E_C) from the Triangle Wave I-V measurements is found to be -5.84 (E_{C-}) and +5.98 (E_{C+}) (+/- 0.1) MV/cm at room temperature (RT) and found to decrease with increasing temperature up to 600 °C. The devices exhibit high remnant polarizations (> 100 μC/cm^2) which are stable at high temperatures. At 600 °C, our devices show 1 million read cycles with On-Off ratio above 1 for > 60 hours. Finally, the operating voltages of our AlScN ferrodiodes are < 15 V at 600 °C which is compatible with Silicon Carbide (SiC) based high temperature logic technology, thereby making our demonstration a major step towards commercialization of NVM integrated high-T computers. NVM characteristics of engineered ferrodiodes with higher On-Off ratios at > 600 °C will also be presented in the meeting.

[a] Dhiren K. Pradhan and David C. Moore contributed equally to this work.

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8:15am **EM+AIML+AP+QS+TF-WeM-2 Oxygen Diffusion Coefficients in Ferroelectric Hafnium Zirconium Oxide Thin Films**, ***Jon Ihlefeld***, *L. Shvilberg,* University of Virginia*; C. Zhou,* North Carolina State University

Just over a decade ago, ferroelectricity – the presence of a permanent reorientable dipole – was reported in doped hafnium oxide thin films. This report generated a great deal of excitement as the inherent silicon compatibility of HfO_2, coupled with the extreme thinness of the films that exhibited the ferroelectric response promised to overcome a number of technological hurdles limiting utilization of ferroelectrics in microelectronics. While the material is moving toward mass production, there are lingering issues of insufficient endurance and limited retention. These issues are commonly attributed to oxygen point defects, including the drift of these defects in poled devices. As such, knowledge of oxygen transport in the ferroelectric phase is vital toward overcoming the current shortcomings. In this presentation, we will show the results of experiments using ^{18}O tracers to evaluate the diffusion coefficient of oxygen in the ferroelectric phase. Hafnium zirconium oxide films containing ^{16}O were prepared via plasma-enhanced atomic layer deposition followed by post-metallization annealing to form the ferroelectric phase. Following removal of the metal layer, an ^{18}O-containing hafnium zirconium oxide film was deposited via thermal atomic layer deposition with ^{18}O provided from a $H_2{}^{18}O$ source. Tracer anneals were then performed and the ^{18}O position evaluated with secondary ion mass spectrometry. The results will show that the oxygen diffusion coefficients in the ferroelectric phase are extremely low, with extrapolated room temperature values of only 10^{-26} cm^2/sec derived. The activation energy for oxygen diffusion was calculated to be 1 eV, which is intermediate the values calculated for the equilibrium monoclinic phase and amorphous films. These results indicate that oxygen vacancies may be relatively immobile in ferroelectric hafnia devices and that other charged defects may be the primary source of degradation.

8:30am **EM+AIML+AP+QS+TF-WeM-3 Thin Film Physics of Ferroelectric HfO_2 and ZrO_2 - From Laboratory Demonstrations to Semiconductor Chips**, *P. Lomenzo,* ***Uwe Schroeder,*** Namlab, Germany **INVITED**

Integrated ferroelectric devices for non-volatile memory applications have been undergoing pioneering developments in recent years due to the CMOS-compatible and highly scalable ferroelectricity exhibited by HfO_2- and ZrO_2-based thin films. A unique hallmark of these industry-friendly ferroelectric materials is the underlying fluorite crystal structure that contains a rich polymorphic landscape in which polar and antipolar crystal phases can be stabilized with unique ferroelectric, pyroelectric, and piezoelectric properties. Obtaining high performance ferroelectric properties for electronic device applications in HfO_2 and ZrO_2 thin films is contingent upon the single-phase formation of the ferroelectric $Pca2_1$ orthorhombic phase, which is challenging due to the competing formations of the nonpolar monoclinic and tetragonal phases. Chemical doping, film thickness, film stress, film growth processing parameters, annealing conditions, defects, and the encapsulating device (i.e., electrodes, interfaces) can all influence the structure and functional electrical behavior of these ferroelectrics.

Due to the extremely scaled film thickness (< 4 nm) and the unique fluorite structure these ferroelectric materials exhibit, tremendous developments in material and device physics have taken place over the past decade. Not only are the underlying intrinsic ferroelectric properties critical for ferroelectric HfO_2- and ZrO_2-based devices, but the interaction between the ferroelectric thin film and the electrodes is much more prominent than conventional, thicker perovskite ferroelectrics. While the coercive field and remanent polarization are nominally determined by the intrinsic film properties of ferroelectric fluorites, extrinsic factors, such as oxygen vacancies and interfacial layers, frequently influence these important ferroelectric parameters that dramatically affect the read/write energy and memory window of ferroelectric random access memory (FeRAM) technologies, respectively. Moreover, reliability challenges such as read/write endurance and retention in both FeRAM and ferroelectric field effect transistors (FeFETs) non-volatile memory technologies involve the intricate coupling between the ferroelectric film, electronically active defects, operation scheme, and the device structure itself.

An in-depth overview is given of current state-of-the-art developments in both the material and device physics of ferroelectric HfO_2 and ZrO_2 thin films. Physical insights obtained from laboratory-scale experiments and devices are compared and contrasted with chip-level demonstrators of non-volatile memories incorporating these novel fluorite ferroelectric thin films.

9:00am **EM+AIML+AP+QS+TF-WeM-5 Iridium Etching: ExploringReactive Ion Etching Parameters for Efficient Electrode Fabrication inFerroelectric Memory**, ***Yanan Li,*** *P. Bezard, S. Kundu, F. Lazzarino, X. Piao, Y. Canvel,* IMEC Belgium

Non-volatile Ferroelectric lead zirconium titanate (PZT) are interesting candidates for future memory applications but the fatigue resistance of the electrode material from the capacitors is a challenge. Iridium (Ir) is being investigated as electrode material for its superior characteristic. Thus, a patterning process must be developed. Due to the low volatility of the etch products, etching Ir is typically performed by ion beam etching (IBE). The low-throughput, relative scarcity of IBE chambers in the industry, as well as the limited tunability of the sputtering process are motivations for the development of a plasma-based etching approach.

In this work, we conducted experiments with TiN as a hard mask, following the process flow shown in Figure 1. Preliminary data indicates that Ir can be etched using both fluorine-based and chlorine-based gases. We identify and highlight the primary parameters affecting the Ir etch rate in the RIE process, focusing on gas flow rates, power settings, pressure, and substrate temperature. We also compare the relative contributions of physical and chemical reactions to the etch rate of Ir.

XSEM pictures for those experiments are shown in figures 2 and 3. It is observed that selectivity with a TiN hard-mask is a challenge when using these chemistries. Sidewall residues have also been observed in conditions where ion sputtering is dominant. Therefore, optimization of the etch processes based upon an understanding of the etch mechanisms in place is necessary.

9:15am **EM+AIML+AP+QS+TF-WeM-6 Investigations in Current Transport Mechanisms of Multi-Resistance State Hafnia Zirconia Ferroelectric Tunnel Junctions**, ***Troy Tharpe,*** Sandia National Laboratories*; M. Lenox,* University of Virginia*; S. Jaszewski, G. Esteves,* Sandia National Laboratories*; J. Ihlefeld,* University of Virginia*; M. Henry,* Sandia National Laboratories

Since the discovery of ferroelectricity in doped hafnia (HfO_2) and alloyed hafnia zirconia thin films $(Hf,Zr)O_2$ over a decade ago, fluorite-structure binary oxides have garnered great interest for use within ferroelectric memory devices to realize compute-in-memory (CiM) and neuromorphic applications. With conformal atomic layer deposition (ALD) techniques, process temperatures below 400 °C, coercive fields close to 1 MV/cm, and ferroelectricity down to ~ 1nm, hafnia thin films are ideal candidates for back-end-of-line (BEOL) integration with complementary metal oxide semiconductor (CMOS) circuits. Leveraging these qualities, recent research has extensively focused on charge-based hafnia devices, such as ferroelectric random access memory (FeRAM) and ferroelectric tunnel junctions (FTJs). FTJs are realized by sandwiching a 4-7nm ferroelectric between electrodes to form a metal-ferroelectric-metal (MFM) structure with a voltage-controlled resistance modulated by polarization. Thinner than FeRAM and able to generate multistate resistances, FTJs are poised to enable energy efficient CiM devices and artificial intelligence (AI) hardware accelerators with improved performance and small form factor.

In this work, we study FTJs with 7 nm thick $Hf_{0.5}Zr_{0.5}O_2$ deposited by plasma enhanced ALD, and asymmetric 20 nm niobium (Nb) / 115 nm niobium nitride (NbN) electrodes deposited by magnetron and reactive sputter, respectively. Film ferroelectricity is stabilized by subsequent anneal at 565 °C for 90s in argon ambient. Fig. 1 (a) depicts an optical image of fabricated HZO FTJs while Fig. 1 (b) illustrates a cross section of device layers. Current density vs voltage (J-V) sweeps are taken at 294, 323, 348, 373, and 398 K for HZO FTJs with diameters varying from 74 µm to 117 µm. Fig. 2 (a) shows these J-V sweeps for a 100 µm diameter device, after application of 10 wakeup cycles. Fig. 2 (b) shows high resistance state (HRS) and low resistance state (LRS) trends across temperature for this same device at 0.2V and 0.3V. Fig. 3 (a, b) shows average and outlier resistance ratio (RR) temperature dependence for 4 devices at 0.2 V and 0.3V, respectively. Fig. 3 (c) depicts pulsed hysteresis curves for a 99 µm diameter device at 294 K and 398 K. Device resistance is read at 0.2V and a pulse width of 100ms, following a write pulse progressing from 1.5V to 1.3V and back with 100mV step and 100ms pulse width. The nonlinear HRS, LRS and RR temperature trends indicate a complex conduction system within HZO FTJs, highlighting the need for continued investigation of current transport mechanics for the realization of ferroelectric CiM devices and multistate AI accelerators.

9:30am **EM+AIML+AP+QS+TF-WeM-7 Correlation between Elastic Modulus and Biaxial Stress in Hafnium Zirconium Oxide (HZO) Thin Films**, ***Megan Lenox,*** University of Virginia*; S. Jaszewski,* Sandia National Laboratories*; S. Fields,* Naval Research Laboratory*; A. Salanova, M. Islam, M. Hoque,* University of Virginia*; J. Maria,* Penn State University*; P. Hopkins, J. Ihlefeld,* University of Virginia

The discovery of ferroelectricity in hafnium oxide based thin films has catalyzed significant research focused on understanding the ferroelectric property origins when fabricated in conventional metal-ferroelectric-metal geometries. Studies have revealed that electrode material selection impacts oxygen vacancies, interfacial layers, and biaxial stress, all noted responsible ferroelectric mechanisms. The coefficient of thermal expansion (CTE) incongruency between the hafnia and the electrode material induces an in-plane tensile stress following post-metallization annealing. However, recent work has shown that while the electrode material CTE does have an effect, the overall strain resulting from the device is primarily from the CTE of the silicon substrate and densification of the hafnia film during crystallization. This notwithstanding, comparisons between electrode materials have shown significant differences in ferroelectric remenant polarization (P_r) behavior. This work describes these polarization differences through the lens of the elastic modulus of the electrode material. TaN/HZO/TaN/*M* devices, where *M* is platinum, TaN, iridium, tungsten, and ruthenium, were fabricated using plasma enhanced atomic layer deposition and sputtering for the hafnia and metal layers, respectively. Wafer flexure measurements done using stylus profilometry revealed each metal electrode material was compressive as deposited. Two-dimensional X-ray diffraction, utilized to derive the $\sin^2(\psi)$ in-plane biaxial stress in the HZO, revealed a strong correlation between stress and electrode elastic modulus (E). Further, Polarization-electric field ($P(E)$) measurements at 2.5 MV cm^{-1} field also showed dependence of $P\text{-}_r$ on measured E. Conversely, no correlation exists between the electrode CTE and P_r or biaxial stress, respectively. Increasing modulus results in a greater resistance to deformation of the electrode, which when deposited prior to annealing the HZO to crystallize from the amorphous state, restricts the out-of-plane expansion of the HZO, promoting the stabilization of the ferroelectric orthorhombic phase, in a phenomenon known as the “capping effect”. This work further promotes the acceleration integration of HZO into MFM devices, such a non-volatile memory devices.

11:00am **EM+AIML+AP+QS+TF-WeM-13 Innovations in DARPA’s Optimum Processing Technology Inside Memory Arrays (OPTIMA) Program**, ***Todd Bauer,*** DARPA **INVITED**

Fast,compact, and power-efficient compute-in-memory (CIM) accelerators can move machine learning from data centers to edge compute devices, enabling training and inference to be done where the training data is collected. However, conventional accelerators that use vonNeumannarchitectureshave poor area and computationalpowerefficiency and longexecutionlatency.CIMarchitectureswithMultiplyAccumulateMacros(MAMs)canaddressthe power and performancelimitationsof approaches that use von Neumann hardware architectures. To date these MAM implementationshavebeenhinderedbythelargephysicalsizeofmemoryelements andthehigh-powerconsumptionofsupportingcircuitry.The Defense Advanced Research Program Agency’s OptimumProcessingTechnologyInsideMemoryArrays(OPTIMA)programseekstodeveloparea-andpower-efficienthigh-performanceMAMswithinnovativesignalprocessingcircuits. The key technical challenges that performers are addressing include 1) developing area-efficient, multi-bit memory elements (i.e. 8 bits of storage in a 1T-1C structure) that can be incorporated into compact multiply compute elements (MCEs) and 2) achieving compact, scalable, and power-efficient MAM circuits. This presentation will provide an overview of the OPTIMA program goals and approaches to achieving those goals.

11:30am **EM+AIML+AP+QS+TF-WeM-15 A Transition Toward Solid-State in TiO_2 Protonic ECRAM**, ***John Hoerauf,*** University of Maryland, College Park*; M. Schroeder,* Army Research Laboratory*; D. Stewart, G. Rubloff,* University of Maryland, College Park

AI and inference learning energy demands are on pace to surpass global energy production[1], but analog in-memory computing hardware can reduce the energy required by up to six orders of magitude[2]. Electrochemical RAM (ECRAM) is a new and promising transistor technology to realize physical neuromorphic analog in-memory computing circuits, achieved on the device level by modifying a thin-film battery stack to measure the impedance of a selected electrode. The impedance is controlled by changing the state of charge of the battery, electrochemically doping the selected electrode with the electrochemically active species. ECRAM that utilizes protons as the electrochemically active species is compatible with existing CMOS devices, has faster programming speed and increased device durability compared to more established Lithium ion ECRAM. As a less well studied system, it is helpful to understand the insertion of protons in and out of the electrode of interest using a more traditional liquid cell before advancing to a solid-state system. In this presentation, the liquid cell electrochemical characteristics and degradation mechanisms in anatase TiO_{-2} are discussed with and without a capping Nafion film. It is observed that the anatase TiO_2 electrode’s typically quick degradation is suppressed by adding a spin-cast Nafion film, increasing cyclability in an aqueous acetate buffer solution by >10x cycles and altering the H^+ insertion kinetics. Subsequently, TiO_2 is used in an all-solid-state three electrode transistor by splitting the bottom current collector into a source-drain configuration and using PdH_x as the counter electrode and H^+ reservoir. Results toward novel solid state anatase TiO_2 based protonic ECRAM are discussed with a focus on device state modulation by electrochemical doping.

[1] B. Bailey, “AI Power Consumption Exploding,” Semiconductor Engineering. Accessed: May 09, 2024. [Online]. Available: https://semiengineering.com/ai-power-consumption-exploding/

[2] E. J. Fuller et al., “Li-Ion Synaptic Transistor for Low Power Analog Computing,”Advanced Materials, vol. 29, no. 4, p. 1604310, 2017

11:45am **EM+AIML+AP+QS+TF-WeM-16 Effects of Gamma Radiation on the Structural and Ferroelectric Properties of Hafnium Zirconium Oxide Capacitors**, ***Samantha Jaszewski,*** Sandia National Laboratories*; M. Lenox, J. Ihlefeld,* University of Virginia*; M. Henry,* Sandia National Laboratories

Ferroelectric hafnium oxide (HfO_2) presents opportunities for technological developments in microelectronics, such as scaling of ferroelectric random-access memory (FeRAM) and new devices such as ferroelectric field-effect transistors (FeFETS) and ferroelectric tunnel junctions (FTJs), that were not previously possible with conventional ferroelectrics. This is due to its compatibility with silicon and ability to exhibit a ferroelectric response in films as thin as 1 nm. Understanding the interaction between radiation and HfO_2-based ferroelectrics is necessary before this material can be utilized in devices facing radiation-hostile environments. In this work, the effects of varying doses of gamma radiation (1 to 8 Mrad) on the structural and electrical properties of metal-ferroelectric-metal capacitors fabricated with 17 nm thick hafnium zirconium oxide (HZO) layers is investigated. Additionally different electrode materials, titanium nitride and tungsten, will be compared. Polarization-electric field, capacitance-voltage, and leakage current measurements were made after electric field cycling with voltages ranging from 2.6 to 4 V. It will be shown that the devices experience decreased endurance and a shift in the coercive voltage that scales with the applied gamma dose and depends on the electrode material. Synchrotron nano-Fourier transform infrared spectroscopy measurements demonstrated that no significant phase changes occur after radiation in these films. This work advances the understanding of the interaction between radiation and HfO_2-based ferroelectrics in order to probe the fundamental limits of radiation tolerance in this material.

12:00pm **EM+AIML+AP+QS+TF-WeM-17 Reconfigurable Ferroelectric Field-Effect Transistor Arrays from SWCNTs**, ***Dongjoon Rhee,*** *K. Kim, S. Song,* University of Pennsylvania*; L. Peng,* Peking University, China*; J. Kang,* Sungkyunkwan University (SKKU), Republic of Korea*; R. Olsson III, D. Jariwala,* University of Pennsylvania

Ferroelectric field-effect transistor (FeFET) is a promising nonvolatile memory device due to its simple and compact device structure for high-density integration, fast switching peed, and non-destructive readout. Recent progress in FeFETs based on two-dimensional (2D) semiconductor channels and ferroelectric $Al_{0.68}Sc_{0.32}N$ (AlScN) has enabled high-performance nonvolatile memory devices with remarkably high ON-state currents, large current ON/OFF ratio, and large memory windows. However, the wafer-scale synthesis of these 2D semiconductors typically demands growth temperatures exceeding 500 °C, rendering the synthesis process incompatible with back-end-of-line (BEOL) processing and necessitating a subsequent transfer step. Solution-based assembly of semiconducting single-walled carbon nanotube (SWCNT) has shown promise as a strategy to fabricate high-quality semiconducting channels at room temperature, but their integration with AlScN for FeFETs has not yet been achieved. In this work, we present a large array of FeFETs utilizing a dense monolayer film of highly aligned semiconducting SWCNTs and ferroelectric AlScN. Our

SWCNT FeFETs can be engineered from *p*-type to ambipolar by changing the contact metals at the metal-semiconducting interface. The ambipolar FeFETs showed high electron and hole current densities, both exceeding 300 μA um^{-1}, along with stable memory retention over 10^4 s and endurance greater than 10^4 cycles. Our devices can also function as reconfigurable *p*- and *n*-FETs by switching the polarization direction of AlScN, potentially enabling multifunctional logic and memory applications at the circuit level.

Quantum Science and Technology Mini-Symposium
Room 123 - Session QS-WeM

Quantum Technologies: From Networks and Education to Sensors and User Facilities

Moderators: Vijaya Begum-Hudde, University of Illinois at Urbana-Champaign, **Sean Jones**, Argonne National Laboratory, **Corey Rae McRae**, National Institute of Standard and Technology

8:00am **QS-WeM-1 The New York Quantum Network: An Advanced Platform for Experiments in Real-Life Conditions***, **Gabriella Carini**,* Brookhaven National Laboratory **INVITED**

The BNL – SBU (Brookhaven National Laboratory – Stony Brook University) team has built one of the longest and most advanced quantum networks now covering more than 161 miles with five distinct nodes on Long Island. The network uses commercial optical fibers and operates at standard telecommunication wavelengths. It includes quantum memories and remote-control capabilities. Research to expand the use of different quantum platforms and network links including free space link for a truly heterogeneous quantum network is ongoing. The team is focused on developing quantum network key technologies as well as novel applications of entanglement distribution network. An overview of the activities will be presented at the conference.

8:30am **QS-WeM-3 Building Quantum Information Science Capabilities at HBCUs: Insights and Recommendation***, K. Lee,* IBM*; M. Lowe,* IBM HBCU Quantum Center, Howard University*; **Thomas A. Searles**,* University of Illinois - Chicago

The IBM HBCU Quantum Center is at the forefront of revolutionizing Quantum Information Science and Engineering (QISE) education and research through a one-of-a-kind industry academic partnership. In this presentation, we delve into various strategies for building Quantum Information Science and Engineering (QISE) capabilities at Historically Black Colleges and Universities (HBCUs), drawing insights from initiatives such as the IBM HBCU Quantum Center while considering the broader context. Our discussion encompasses the current status of QISE initiatives at HBCUs, including curriculum development, research capabilities, and faculty demographics across physics, computer science, and engineering departments.

We explore the interdisciplinary nature of quantum education and research, emphasizing collaborative efforts aimed at equipping students with the skills necessary for success in advanced computing technologies of the future. Drawing upon the experiences and achievements of HBCUs involved in quantum initiatives, we offer actionable recommendations for enhancing capacity-building efforts. These recommendations encompass curriculum enhancement, faculty recruitment and retention strategies, research collaboration frameworks, and initiatives to promote diversity and inclusion across disciplines.

In conclusion, this presentation provides a comprehensive overview of the ongoing efforts to build QISE capabilities at HBCUs, informed by both specific initiatives such as the IBM HBCU Quantum Center and broader trends within the HBCU community. Through collaboration and strategic investment, we can further advance quantum education and research, ensuring that HBCUs play a pivotal role in shaping the future of quantum information science.

8:45am **QS-WeM-4 The UCSB NSF Quantum Foundry***, **John Harter**,* UC Santa Barbara **INVITED**

Founded through the NSF's Q-AMASE-i initiative, the Quantum Foundry at UC Santa Barbara is a next generation materials foundry that develops materials and interfaces hosting the coherent quantum states needed to power the coming age of quantum-based electronics. The mission of the Foundry is to develop materials hosting unprecedented quantum coherence, train the next generation quantum workforce, and to partner with industry to accelerate the development of quantum technologies. In this talk, I will present a broad overview of the activities and services of the UCSB NSF Quantum Foundry over the last several years.

9:15am **QS-WeM-6 Recent Progress in Quantum Applications via the Q-One Single Ion Implantation System***, **Gianfranco Aresta**, K. Stockbrodge,* Unit B6, UK*; K. McHardy, P. Blenkinsopp,* Ionoptika Ltd., UK

Quantum computing has the potential to revolutionize many aspects of modern technology, including digital communications, “quantum-safe” cryptography, and incredibly accurate time measurements. The development of this technology represents the next great frontier of science and engineering.

Devices based on single impurity atoms in semiconductors are receiving attention as potential quantum technologies and shown to be promising proof-of-concept.

However, such devices are incredibly challenging to manufacture, as single atoms must be placed within nanometric precision in isotopically pure host matrix such as ^{28}Si.

All working devices thus far have been fabricated using hydrogen lithography with an STM followed by atomic layer deposition. This is labor-intensive and requires several days of meticulous preparation to create just a single quantum bit (qubit).

Real-world devices will require arrays of hundreds or thousands of impurity atoms, highlighting the requirement for a scalable method of positioning single atoms with nanometer precision.

In 2019, Ionoptika launched a new commercial focused ion beam (FIB) instrument specifically made for the fabrication of quantum materials and devices via single ion implantation, the Q-One.

With a continuously expanding range of available ion species, a high-resolution mass-filter system, high-precision stage and proven capability of single ion deterministic implantation with isotopic resolution, Q-One is, nowadays, the instrument of choice for Universities and Research Institutes.

During last year’s AVS Conference we reported on the overall Q-One performances and Liquid Metal Alloy Ion source development carried out at Ionoptika, since the instrument launch.

This year we will report on the results achieved with the Q-One instrument by different research groups. Due to the fact that the ion dose delivered to the sample can be adjusted across a wide range, providing many nanoscale material engineering capabilities in a single tool, examples of the Q-One use as a photolithographic tool, to achieve a ^{28}Si matrix, and single ion implantation will be reported and discussed.

9:30am **QS-WeM-7 Laying the Foundation for a Global Quantum EconomyThrough Sensors and Standards***, **Barbara Goldstein**,* NIST **INVITED**

Bringing quantum technologies out of the lab and into the market requires a new foundation of metrology and standards. Quantum 2.0, which exploits properties like superposition and entanglement, presents a new suite of parameters to measure, requires the characterization of components in new environments such as at cyrogenic temperatures, and challenges us to come up with benchmarks that work across multiple and rapidly changing hardware platforms, such as for quantum computing and networking. This talk will explore the role of standards in critical and emerging technologies, how the broader quantum community is working together to develop pre-standards (NMI-Q) and standards (IEC/ISO JTC-3), and will provide an overview of the NIST on a Chip program which is developing a suite of intrinsically accurate, fit-for-function quantum-based sensors and standards.

11:00am **QS-WeM-13 PARADIM: An NSF-Supported National User Facility that can help YOU Discover and Perfect Quantum Materials***, **Darrell Schlom**,* Cornell University **INVITED**

Creating quantum materials with unprecedented properties, by design rather than by serendipity, is accomplished in PARADIM through a synergistic set of user facilities dedicated to theory, synthesis, and characterization. Each of these world-class user facilities is equipped with the latest tools, techniques, and expertise to help users like you realize this materials-by-design dream. Users from throughout the nation are using PARADIM to discover and create quantum materials.*

PARADIM’s vision is to democratize materials discovery in the U.S.A. and to enable a more effective way of pursuing materials research, one that accelerates materials discovery by establishing a materials discovery ecosystem—a national community of practitioners—and equipping them

with theoretical and experimental methods that enable them to reduce to practice the inorganic materials of which they dream. Among the tools that PARADIM provides it users are:

• A fully automated MBE system in which users can select among 62 elements of the periodic table and grow at substrate temperatures as high as 2000 °C—the most elements and the hottest growth temperatures of any MBE system in the world—to make the inorganic materials desired. Any 11 of these elements may be loaded into the MBE system at one time.

• An *in situ* UHV connection between PARADIM's 62-element MBE system and a spin-resolved ARPES system enabling users to determine the electronic structure of the new materials and interfaces they create.

• A scanning transmission electron microscope that has achieved the highest resolution ever reported (0.16 Å). This is made possible by a new electron microscope pixel array detector (EMPAD), developed at Cornell, and made available first in PARADIM's electron microscopy user facility.

Use of PARADIM facilities and associated user facilities at Cornell and Johns Hopkins is free to users from academia and national labs from the U.S.A. provided their 2-page proposal is highly ranked by PARADIM's User Proposal Review Committee. All data from PARADIM facilities is recorded and stored for future use. After a period of inactivity or completion of scientific publications by the primary users, all data associated with user projects is made publicly available. PARADIM is also open to users from industry, who pay for access to PARADIM user facilities, but whose data are never made public.

*The capabilities and success stories described in this talk made use of the facilities of the *Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials* (PARADIM), which are supported by the National Science Foundation under Cooperative Agreement No. DMR-2039380.

Electronic Materials and Photonics
Room 114 - Session EM+2D+AP+QS+TF-ThM

Epitaxy: Advances in Materials Integration and Devices

Moderators: Haozhe Wang, Duke University, **Jason Kawasaki**, University of Wisconsin - Madison

8:00am **EM+2D+AP+QS+TF-ThM-1 Electronic and Photonic Integrated Devices Enabled by Local III-V on Si Heteroepitaxy**, *M. Scherrer,* IBM Research GmbH, Zurich Research Laboratory, Switzerland; *K. Moselund,* Paul Scherrer Institute, Switzerland; ***Heinz Schmid,*** IBM Research GmbH, Zurich Research Laboratory, Switzerland

Heterogeneous integration of electronic chiplets is one of the key performance drivers in today's HPC and consumer products. Similarly, a performance benefit can be envisioned by heterogeneous integration of preferred materials at the device level. Here we explore this bottom-up path and report on local growth of III-V compound semiconductors on silicon for electronic and photonic applications. For electronic applications the high charge carrier mobility in III-V materials is particularly interesting, while for optical devices, the direct bandgap and in-plane coupling to Si waveguides are key benefits. We will detail the epitaxial growth of III-Vs on Si by template-assisted selective epitaxy using MOCVD and highlight this method´s uses by discussing selected device characteristics for field-effect transistors [1] and pin photodetectors directly integrated to Si waveguides [2]. The dense and precise co-placement of III-V gain material with Si allows for novel device designs, which will be illustrated by recent results on lasers based on hybrid III-V/Si photonic crystal cavity designs [3].

This research is supported by EU Grant 860095, 678567, 735008 and SNF grant 188173.

[1] C. Convertino et al. Nat. Electron. (2021) doi.org/10.1038/s41928-020-00531-3

[2] P. Wen et al. Nat. Comm. (2022) doi.org/10.1038/s41467-022-28502-6.

[3] M. Scherrer et al. ACS Photonics (2024) doi.org/10.1021/acsphotonics.3c01372

8:15am **EM+2D+AP+QS+TF-ThM-2 In situ Graphene Barriers for Remote Epitaxy of SiC**, ***Daniel Pennachio,*** *J. Hajzus, R. Myers-Ward,* US Naval Research Laboratory

Remote epitaxy (RE) is a thin film growth technique where epitaxial alignment is directed by interactions with a substrate despite it being covered by a top layer of material.[1] This top layer must be inert and atomically thin for the underlying substrate's potential field to dominate the epitaxial alignment. Since the intermediate layer is inert, the epitaxial thin film is weakly bonded to the substrate and can be removed as a freestanding membrane and the substrate can be reused, without the damage associated with other transfer techniques such as controlled cleaving or ion implantation. Transferred 2D two-dimensional (2D) material, such as graphene, is commonly used for a layer, but the transfer can degrade the film and increase process complexity. To avoid this, we aim to grow in situ graphene in the same chemical vapor deposition (CVD) RE growth as SiC. RE SiC is advantageous since the high cost of SiC makes substrate reuse appealing and isolated SiC membranes are excellent for quantum photonics. Despite these benefits, SiC's high-temperature hydrogen-containing CVD environment can easily damage graphene, making RE difficult.

This study established growth windows for in situ graphene via propane-based hot wall CVD followed by subsequent SiC deposition. Growing at 1620 °C in 20 slm H2 with 20 sccm propane flow produced predominantly monolayer (ML) graphene films on on-axis 6H-SiC(0001) substrates and 2-3 ML films on 4° off-axis 4H-SiC(0001) substrates with minimal defects found in Raman spectral maps. These films exhibited increased uniformity over graphene grown via Si sublimation from the SiC substrate, as determined by atomic force microscopy (AFM) and Raman spectral maps. This optimal graphene growth condition was used for subsequent RE attempts to study the effect of SiC growth temperature, precursor C/Si ratio, and growth rate on epilayer crystallinity and graphene barrier damage. Nomarski microscopy, scanning electron microscopy (SEM), and AFM found SiC grown at 1620°C with a C/Si ratio of 1.55 to have the smoothest surface morphology and fewest polytype inclusions. SiC crystalline quality appeared correlated to growth rate, with lower growth rates producing smoother films with fewer polytype inclusions. Single-crystalline, polytype-pure SiC epilayers was achieved on 4° off-axis CVD graphene/4H-SiC(0001). Cross-sectional transmission electron microscopy (TEM) of some growth interfaces in this study exhibited non-uniform multilayer graphitic carbon, motivating further study of this growth system to improve boundary uniformity and SiC epilayer quality.

[1] Kim, Y., Cruz, S., Lee, K. et al. Nature 544, 340–343 (2017).

8:30am **EM+2D+AP+QS+TF-ThM-3 Basal Plane Dislocation Mitigation via Annealing and Growth Interrupts**, ***Rachael Myers-Ward,*** *N. Mahadik, D. Scheiman, J. Hajzus, S. White, D. Pennachio,* Naval Research Laboratory

Basal plane dislocations (BPD) in SiC are high-voltage bipolar device killers that source Shockley-type stacking faults in the presence of an electron-hole plasma [1].Multiple research groups have been successful in mitigating their propagation from the substrate into the epitaxial layer [2-5]. While these are sufficient for typical SiC devices, for high pulsed power current density or high surge current capability applications, the injected carrier concentration is significant enough to expand converted BPDs. Here, we will report results from comparisons of H_2 etching to Ar annealing and the use of H_2 versus Ar during growth interrupts to prevent BPD expansion.

SiC epitaxial layers were grown using a CVD reactor on 4° off-axis substrates toward the [11-20] that are known to have BPDs. A H_2 etch or Ar anneal was performed before the buffer layer (BL) growth while a growth interrupt in H_2 or Ar was conducted prior to the intentionally low doped drift layer. Ultraviolet photoluminescence (UVPL) imaging was used to image the samples before and after UV stressing up to 13 $kWcm^{-2}$.

The H_2 etch and H_2 growth interrupt prevented BPDs from expanding under UV stress of 13$kWcm^{-2}$ and it is believed that the H_2 treatment specifically inhibited this expansion. To confirm the role of H_2, we performed a growth using the same conditions as the H_2 etch/interrupt, however, an Ar anneal was used instead of a H_2 etch and the growth interrupt was conducted in an Ar atmosphere instead of H_2. The sample was UV stressed up to 1000 Wcm^{-2} and it was found that four BPD expanded from the substrate into the epilayer. For comparison, a sample grown with a double H_2 etch (before the buffer layer growth and drift layer) and a sample grown with a H_2 etch plus H_2 growth interrupt did not produce faulting at the same power density. This indicates that H_2 influences BPD expansion. We will present detailed parametric results of samples grown with various etching/ annealing, growth interrupts, anneal times, buffer layer thickness, gas flow rates and interrupt temperature, both in H_2 and Ar.

[1]J.P. Bergman, *et. al.*, Mater. Sci. Forum Vol. 353-356, 299 (2001).

[2]N.A. Mahadik *et.al.*, Mater Sci Forum 858, 233 (2016).

[3]R. E. Stahlbush, et *al.*, Appl. Phys. Lett. 94, 041916 (2009).

[4]M. Kato, *et al.*, Sci. Rep., 12, 18790 (2022).

[5]N.A. Mahadik *et. al.*, Appl. Phys. Lett., 100, 042102 (2012).

8:45am **EM+2D+AP+QS+TF-ThM-4 Shadow Mask Molecular Beam Epitaxy**, *S. Mukherjee, R. Sitaram, X. Wang,* University of Delaware; ***Stephanie Law,*** Pennsylvania State University

Shadow mask molecular beam epitaxy (SMMBE) is a form of selective area epitaxy (SAE)which uses a mask either directly fabricated on or placed in contact with the substrate. During film deposition, epitaxial layers are grown on the substrate through apertures in the mask. In addition to selective area growth, SMMBE also produces a shadowing effect near the mask edges in which elemental fluxes vary as a function of position. This results in a gradient of film thickness and/or composition near the mask edges. The steepness of the gradient can be controlled by varying the mask thickness and/or the angle of the mask edges. In this paper, we demonstrate the potential of the SMMBE technique to create in-plane gradient permittivity materials (GPMs) by taking advantage of the shadowing effect. A GPM is a material in which the permittivity varies as a function of location. Our aim is to synthesize in-plane GPMs, in which the permittivity varies in the lateral in-plane direction rather than in the vertical growth direction. In an in-plane GPM, different wavelengths of light can be confined at different in-plane locations on the chip. We are interested in creating an infrared GPM, so we chose Si:InAs as our material. To create our GPMs, we use the SMMBE approach: by creating flux gradients of both indium and silicon near the edges of the mask, we can control the doping density and thus the permittivity of Si:InAs in the lateral in-plane direction. We started with reusable Si masks that are 200 um thick and 1 cm x 1 cm in dimension. Each mask has an aperture at its center which has a dimension of 0.5 cm x 0.5 cm at the top and 0.528 cm x 0.528 cm at the bottom. Nano-FTIR spectra obtained via s-SNOM using a mid-IR nano-FTIR module demonstrates that we successfully synthesized infrared GPMs. The GPM grown using a 200 um mask can confine light with wavenumbers 650 cm^{-1}

to 900 cm^{-1} over an in-plane distance of 13 um. In this talk, I will discuss the influence of several growth parameters in controlling the in-plane permittivity of the GPMs, including the growth temperature, mask thickness, and As:In ratio. In particular, the 500 um mask provides a larger shadowing effect in comparison to 200 um mask. This leads to a larger gradient in permittivity over a longer in-plane distance in the GPM: light with wavenumbers 650 cm^{-1} to 1400 cm^{-1} can be confined over an in-plane distance of 30 um. This provides a larger surface area for the construction of an ultracompact spectrometer. Tailored mask designs can be employed to synthesize in-plane GPMs with tailored permittivity gradients in the future.

9:00am **EM+2D+AP+QS+TF-ThM-5 Impact of Excess Ga on Electronic Properties in Plasma-assisted MBE-grown β-Ga_2O_3**, ***Thaddeus Asel,*** *B. Noesges, J. Li, Y. Kim, A. Neal, S. Mou,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

β-Ga_2O_3 has been of significant interest due to its high electric breakdown field, commercially available native substrate, and shallow n-type donors. However, β-Ga_2O_3 differs from other Ga-based semiconductors where metal-rich growth conditions are utilized to achieve adsorption-controlled growth by consuming the Ga flux entirely. Instead, β-Ga_2O_3 growth must balance the incorporation of Ga with the desorption of a volatile suboxide species, Ga_2O where this suboxide is a limiting step when growing β-Ga_2O_3 via molecular beam epitaxy (MBE) with a traditional Ga source. Increased Ga_2O desorption causes the growth rate of β-Ga_2O_3 to decrease as the Ga flux is increased beyond the stoichiometric point of the material and can impact the stoichiometry of the grown film. In this work, we explore the impact of O-rich and Ga-rich conditions on electronic properties in films of β-Ga_2O_3 grown via plasma-assisted MBE (PAMBE). Initial results comparing two samples under O-rich and Ga-rich conditions showed a large difference in peak low-temperature mobility. The O-rich sample showed a peak low temperature mobility of 793 cm2 /V·s while Ga-rich sample peaked at only 198 cm2 /V·s. The mobility and volume carrier density versus temperature data was fit using a model to extract out donor and compensating acceptor density. The Ga-rich sample showed an acceptor concentration of 2.0×10^{16} cm^{-3} compared to the O-rich sample that was measured to have an acceptor concentration of 3.0×10^{15}, and order of magnitude lower. This is possibly due to the formation of V_{Ga} during the Ga_2O desorption process during the growth of the films. Another series of films were grown across a wider range of O- to Ga-rich conditions to further establish a trend between growth conditions and compensating acceptor density. Only Ga flux varied between samples and substrate temperature, Si source temperature and RF oxygen plasma conditions were held constant. Si concentration in each film was anti-correlated with the growth rate which is expected. Conversely, compensating acceptor density increased with increasing Ga-rich conditions and does not follow the trend of the growth rate. The best peak low-temperature mobility occurred for the sample grown in the most O-rich conditions (789.6 cm^2/Vs) and mobility decreased with increasing compensating acceptor concentration. Overall, these results indicate the importance of Ga:O ratios in β-Ga_2O_3 films grown via MBE with conventional Ga sources. These results demonstrate how improved electronical performance can be achieved in β-Ga_2O_3 by growing under O-rich conditions and limiting the formation of V_{Ga} due to suboxide desorption.

9:15am **EM+2D+AP+QS+TF-ThM-6 Advancing Single-Crystalline Oxide Membrane Growth via Molecular Beam Epitaxy**, ***Shivasheesh Varshney,*** *S. Choo,* University of Minnesota*; M. Ramis,* Institute of Materials Science of Barcelona (ICMAB-CSIC), Spain*; L. Thompson, J. Shah, Z. Yang, J. Wen, S. J. Koester, K. Mkhoyan, A. S. McLeod,* University of Minnesota*; M. Coll,* Institute of Materials Science of Barcelona (ICMAB-CSIC), Spain*; B. Jalan,* University of Minnesota

A sacrificial layer method has proven to be an effective route for synthesizing free-standing membranes. In this approach, a crystalline sacrificial layer is selectively dissolved in water, allowing the target film to be transferred onto a host substrate. However, commonly used sacrificial layers (such as $SrCa_2Al_2O_6$) have complex stoichiometry, posing synthesis challenges in molecular beam epitaxy (MBE). In this presentation, we will discuss two distinct but MBE-friendly, fast and facile approaches to synthesize single-crystalline oxide nanomembranes using hybrid MBE [1,2]. In particular, we synthesize epitaxially, single-crystalline $SrTiO_3$ membranes, ranging from a few unit cells to several hundred nanometers in thickness, using an SrO sacrificial layer, and a solution-processed amorphous $SrCa_2Al_2O_6$sacrificial layer. Films grows in a layer-by-layer growth mode on a solution-processed amorphous $SrCa_2Al_2O_6$ whereas in a step-flow growth mode on SrO sacrificial layer. Films grown on SrO layer dissolve rapidly (< 5 minutes) in water, resulting in millimeter-sized membranes. Combining structural characterization using x-ray diffraction (XRD), atomic force microscopy (AFM), piezo force microscopy (PFM), and scanning transmission electron microscopy (STEM), we will present the structure-property relationships in these membranes with particular emphasis on investigating the role of non-stoichiometry on dielectric properties. Using PFM, we demonstrate that Sr-deficient films exhibit robust polarization at room temperature, while stoichiometric films remain consistent with the paraelectric phase. Finally, we will present the growth of single crystalline complex oxide films on a compliant substrate consisting of a few unit-cell $SrTiO_3$ seed layers onto an amorphous SiO_2 wafer.

1. S. Varshney, S. Choo, L. Thompson, Z. Yang, J. Shah, J. Wen, S. J. Koester, K. A. Mkhoyan, A. McLeod, and B. Jalan, **"Hybrid Molecular Beam Epitaxy for Single Crystalline Oxide Membranes with Binary Oxide Sacrificial Layers"** *ACS Nano* 8, *18,* 6348-6358 (2024).
2. S. Varshney, M. Ramis, S. Choo, M. Coll, and B. Jalan, "**Epitaxially Grown Single-Crystalline $SrTiO_3$ Membranes Using a Solution-Processed, Amorphous $SrCa_2Al_2O_6$ Sacrificial Layer"** under review (2024) http://arxiv.org/abs/2405.10464

2D Materials

Room 122 - Session 2D+EM+QS-ThA

2D Materials: Applications

Moderators: Matthias Batzill, University of South Florida, **Fei Yao**, University at Buffalo

2:15pm **2D+EM+QS-ThA-1 Tuning Functionality: Graphene Oxide (GO)/Few Layers Graphene (FLG) Membranes for Water Treatments**, *J. Flores-Arciniega, S. Acosta, H. Ojeda-Galván,* CICSaB, Universidad Autónoma de San Luis Potosí, Mexico*; B. Yáñez-Soto,* Instituto de Física, Universidad Autónoma de San Luis Potosí, Mexico*; **Mildred Quintana**,* Facultad de Ciencias, CICSaB, Universidad Autónoma de San Luis Potosí, Mexico

Graphehe oxide (GO) and few layer graphene (FLG) are exciting platforms with a huge potential for developing new advanced technologies. The unique combination of properties, such as high specific surface area, charge transport, chemical stability, mechanical strength, flexibility, high electrical and thermal conductivity, make them the ideal substrates for several applications in water remediation. Here, I will describe the synthesis and processing of GO and FLG, their characterization, handling, and performance towards advanced membranes for water treatments. In particular, we aim to address the production of van der Waals heterostructures for the development of micro and nanofiltration membranes for bacteria removal, organic molecule adsorbents, and desalination. The properties of 2D materials modulate mechanical and chemical stabilities, while active sites are created by the effective construction of van der Waals heterostructures allowing charge and mass transfer producing cost-effective and highly efficient membranes for water purification.

Acknowledgments

CONAHCYT basic science project CB-A1S-8817 and Sinergía-UNAM 1564464, JF thanks to CONAHCYT for Ph.D. scholarship No. 744836. The authors want to thank Laboratorio Nacional de Ingeniería de la Materia Fuera de Equilibrio (LANIMFE), for the use of equipment and technical support.

2:30pm **2D+EM+QS-ThA-2 New Graphene Oxide-based Nanozymes for Cancer Theranostics**, *A. Foti, S. Sciacca, G. Tranchida, S. Petralia, R. Fiorenza, S. Scirè, L. D'Urso, C. Bonaccorso, A. Fraix,* University of Catania, Catania, Italy*; A. De Bonis,* University of Basilicata, Italy*; **Cristina Satriano**,* University of Catania, Catania, Italy

Graphene oxide (GO) and plasmonic nanoparticles (Pd, Au, Ag NP) nanocomposites were scrutinized in this study as combinative multimodal platform with enzyme-like, photocatalytic and photothermal properties. A green one-pot chemical reduction method by using D-glucose as reducing agent and polyvinylpyrrolidone (PVP) as capping agent, was used to fabricate the hybrid 2D platforms (NP@G) and the reference plasmonic nanoparticles alone. Different molar ratios of the metal precursor/reducing agent were tested to get the best results in terms of stability, reproducibility and reaction yield, as monitored by the plasmonic band of the NPs. The physicochemical characterization of the morphological, compositional, structural, and functional properties of NP@G nanozymes was carried out in terms of X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), transmission electron microscopy (TEM), UV-visible, Raman spectroscopy, Fourier Transformed Infrared Spectrocopy (FTIR), thermocamera, atomic force microscopy (AFM), dynamic light scattering (DLS) and zeta potential (ZP). The enzyme-like activity was tested by colorimetric assays in a cell-free environment to confirm the maintenance of the nanozymes capability in the NP@G samples.The photocatalytic properties were tested in the H_2 evolution by water splitting reaction under simulated solar light. Further, the nanoplatforms were tested in prostate cancer cells (PC-3 line) in terms of cytotoxicity, cell migration and reactive oxygen species (ROS) production, to prove the antitumoral action of the developed nanomedicine. Cell imaging by laser scanning confocal microscopy (LSM) demonstrated the theranostic capability of the developed platforms, including dynamic processes at the level of sub-cellular compartments.

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

2:45pm **2D+EM+QS-ThA-3 Graphene and Copper Nanoparticles Based Electrochemical Sensors for the Detection of Glyphosate in Water**, ***Uswah Yasin***, *F. Torrisi,* University of Catania, Italy

Glyphosate is commonly used as a herbicide to control weeds in agricultural and non-agricultural applications (Carretta, et al. J. Chromatography. A 1600, 2019), resulting in significant adverse impacts on the environment, especially contaminated soil and water, with potential effects on human health (Richmond, AESS 8, 2018). Such environmental threat recently triggered the development of enhanced and scalable glyphosate sensing technologies.

Commercial sensors for glyphosate based on gold nanoparticles (AuNPs), silver nanoparticles (AgNPs), quantum dots, show a sensitivity ranging from 0.88 µM to few pM (Zúñiga, et al. Water 14, 15, 2022). Graphene is an excellent material for sensing applications (Fenech-Salerno, et al. Nanoscale 15, 7, 2023) (Schedin, et al. Nat. Mater 6, 9, 2007). Due to the high mobility, large surface area, high mechanical strength, and chemical stability, graphene provides a versatile platform for the detection of a wide range of analytes, including glyphosate. For the detection of glyphosate, graphene-based sensors can achieve a high sensitivity of the order of 0.30×10^{-12} M (Gonçalves, et al. Mater. Today Commun. 36, 2023). In addition, graphene inks enable a large range of printed, sustainable and flexible devices (Carey, et al. Nat. Commun. 8,1, 2017).

Here, we present the preparation of a glyphosate sensor based on graphene and Cu nanoparticles, deposited by a scalable spray-coating process on flexible substrate, such as polyimide (PI) and polyethylene terephthalate (PET). The graphene ink is prepared by liquid phase exfoliation, reaching a graphene concentration of ~ 0.7 mg/ml. The spray-coated graphene ink resulted in electrodes with a sheet resistance of ~ 240 Ω/□, subsequently spray coated with Cu nanoparticles synthesized using Pulsed Laser Ablation in Liquid (PLAL), with the concentration of 12.5 µg/ml, to form the Graphene/Cu nanoparticle (G:Cu) electrode.

The concentration of glyphosate was determined by Multiple Cyclic Voltammetry (CV) using the G:Cu electrode as the working electrode in a glass electrochemical cell loaded with a solution of glyphosate was prepared in Milli-Q water. The CV curve of G:Cu showed the presence of a redox reaction related to the oxidation states of copper ($Cu \rightarrow Cu^{2+}$), compared to a plain graphene electrode, thereby affirming the sensing efficacy of the glyphosate sensor.

Our G:Cu sprayed sensor offers a flexible, sustainable, and scalable solution to detect glyphosate with excellent selectivity and sensitivity making it the perfect approach to address the need for accurate and efficient monitoring of glyphosate contamination in environmental and agricultural settings.

3:00pm **2D+EM+QS-ThA-4 Engineering Novel Hybrid Membranes for Battery Separators from Sustainable Sources**, ***Suvash Ghimire***, *P. Makkar, M. Islam, K. Mukhopadhyay,* University of Central Florida

The surge in device use in transportation, biomedical sectors, and other industries is escalating at an alarming rate, coupled with grave concerns about pollution and global warming that underscores the urgency for developing efficient, safe, and environmentally friendly energy storage devices. There is a growing urgency to reduce planet-warming pollution through mining and other activities at the federal level to drop carbon emissions by half this decade and reach close to zero by the middle of the century to prevent some of the most devastating effects of climate change. Research groups worldwide are developing metal-based substitutes that address sustainability by eliminating the use and generation of hazardous substances during the synthesis and developing cheap, recyclable substitutes for electrode materials, electrolytes, membranes, and separators that are the pivotal components of energy storage devices.

Materials and their interfaces play an essential role in energy storage devices by facilitating ion transports and impeding short circuits by separating anode and cathode. Ion exchange membranes have broad applications in water electrolysis, fuel cells, and flow batteries. To date, Nafion® membranes and polyolefin-based separators are considered the industrial standards due to their excellent proton conductivity and high chemical stability. However, high cost, poor strength, shrinkage at high temperatures, and use of fluorinated chemicals hinder their widespread use. Therefore, there is an urgent need to develop membranes that can be alternatives to existing membranes without compromising the cost and environmental impact. Leveraging their porosity, properties, low cost, and thermal and chemical stabilities, clay-based membranes could be a new alternative for new-generation materials for such applications.

Our research presents a novel pathway for developing flexible and durable hybrid clay membranes by modifying them with zwitterions. The ionic conductivity of the membranes, measured using electrochemical impendence spectroscopy in a non-aqueous electrolyte solution, was found to be in the range of 10^{-4} S/cm, which is comparable to the ionic conductivities of related membranes used in electrochemical energy storage devices; this is a significant new development considering clays are insulators. Our study exhibits a new avenue to engineer highly efficient ion-conducting membranes with high thermal stability (300 °C) that can provide an efficient and recycle-free approach to developing a new generation of separators from sustainable sources for energy applications, especially for battery technology.

3:15pm **2D+EM+QS-ThA-5 Unveiling Composition-Structure Relationships for the Discovery of Novel High-Entropy 2D Materials Using the Mixed Enthalpy-Entropy Descriptor**, ***Dibyendu Dey,*** University of Central Florida*; O. Ogunbiyi,* University of Missouri*; B. Ball,* University of Central Florida*; L. Liang, M. Zachman,* Oak Ridge National Laboratory*; Y. Yang,* University of Missouri*; L. Yu,* University of Central Florida

High-entropy two-dimensional materials (HE-2DMs) represent an emerging class of materials that show promise for numerous functional applications. These materials inherit the distinctive features of conventional 2D materials, such as reduced dimensionality, exceptional flexibility, and a large surface-to-volume ratio, while introducing a high configurational entropy of mixing to the system. Despite their immense potential, the experimental realm of HE-2DMs has thus far been limited to a few materials, leaving the complex interplay between their composition, structure, and synthesizability largely unexplored. In this work, by utilizing the Mixed Enthalpy Entropy Descriptor (MEED) [**1**], the material space of high-entropy 2D chalcogenides, including Group IV (Ti, Zr, Hf), Group V (V, Nb, Ta), and Group VI (Cr, Mo, W) metals in their 2H, 1T, and 1T' phases, has been systematically explored. MEED uniquely encapsulates the chemical and structural attributes critical for synthesizing HE-2DMs in their diverse polymorphs, demonstrating capabilities beyond any existing descriptor. Guided by MEED predictions, several top-candidate high-entropy tellurides and selenides, which exhibit extraordinary potential for applications in flexible electronic devices and advanced batteries, have been synthesized.

Acknowledgments: This work is supported by the US Department of Energy (DOE) Basic Energy Sciences (BES) under Award Number DE-SC0021127.

Reference:

1. Dibyendu Dey, Liangbo Liang, Liping Yu, Journal of the American Chemical Society 146, 5142 (2024).

3:30pm **2D+EM+QS-ThA-6 Antenna-Coupled Magic-Angle-Twist-Graphene Josephson Junction Millimeter Wave Detector**, ***David Castro,*** University of Central Florida

We designed a sensitive detector of THz and mm waves using an antenna-coupled magic-angle-twist-graphene Josephson junctions. Magic angle twisted bilayer graphene superconducts at a transition temperature of ~2K. We can create a lateral Josephson junction by selectively gating different sections of a single sheet of magic angle graphene. The detection mechanism in our design is based on the change in maximum zero-voltage DC current in response to an applied AC signal at the junction. We expect it to be faster than bolometric detection mechanisms while maintaining high sensitivity. We determined that the bowtie antenna would work best for this device by using finite element electrodynamic simulations. We estimated the responsivity, noise-equivalent-power, and the prospects for single-photon detection. This detector device can be used in the future for sensing applications and quantum information systems.

Acknowledgments

This work was supported by U. S. Army OSD Phase II STTR contract W911NF23C0027 and bymatching funds from the Florida High Technology Corridor (I-4) Program.

3:45pm **2D+EM+QS-ThA-7 Antenna-Coupled Graphene Josephson Junction THz/mm-wave Detector**, ***Rachid Ben Khallouq,*** University of Central Florida

We will discuss design, manufacturing processes, response characteristics, and tolerance to twist-angle variations of antenna-coupled Josephson-junction detectors fabricated from magic angle graphene tailored for detecting mm-wave and THz radiation. We find that Josephson junctions realized in magic angle graphene exhibit exceptionally high dynamic resistance at the peak zero-voltage current. When a small microwave voltage is applied across the junction, it induces a change in the voltage-current correlation, resulting in a notable DC output voltage. External radiation can energize a suitable antenna, generating the required AC voltage across the junction. These detectors operate via a non-thermal mechanism, offering the potential for both speed and sensitivity. They display a bolometric response, with an estimated temperature coefficient of resistance of 300%/K. We will show different designs and detection mechanisms and compare them to other technologies.

This work was supported by U. S. Army OSD Phase II STTR contract W911NF23C0027 and bymatching funds from the Florida High Technology Corridor (I-4) Program.

Quantum Science and Technology Mini-Symposium
Room Central Exhibit Hall - Session QS-ThP

Quantum Science and Technology Mini-Symposium Poster Session

Moderators: Andre Schleife, University of Illinois at Urbana-Champaign, **Ekta Bhatia**, NY CREATES

QS-ThP-1 Characterization of Planar Ta Damascene Resonators for Quantum Information Science Applications, ***Drew Rebar***, *F. Ponce, B. VanDevender, M. Warner, J. Macy,* PNNL*; T. Nanayakkara, C. Zhou, M. Liu,* Brookhaven National Laboratory*; S. Papa Rao,* NY CREATES*; E. Bhatia,* SUNY POLY, Albany

Transmon qubits are one of the leading technologies for quantum information science (QIS) with fabrication and characterization techniques accessible by numerous laboratories around the world.In recent years, efforts at coherence time optimization have shifted focus to the performance of the underlying superconducting material and accompanying surface oxides.While earlier devices were fabricated from Al and Nb, the current state-of-the-art transmons are fabricated from Ta with coherence times up to 0.5 milliseconds.Our research focuses on Ta coplanar waveguide (CPW) resonators fabricated by a damascene technique which yields pristine metal structures entrenched in silicon substrates.While the participation ratio of the dielectric substrate is increased, the device edges remain oxide free from the entrenchment and a nitride capping layer.Our recent studies revealed a current best Q value on the order of 105 at low power.This work, performed in collaboration with NY CREATES/SUNY Poly and BNL, will be discussed along with the prospect of further improvements.

QS-ThP-2 DNA-Enabled Precise Arrangement of Colloidal Quantum Dots and Rods on Device Substrates, ***Xin Luo***, *C. Chen, M. Bathe,* MIT

Colloidal quantum dots (QDs) and rods (QRs) are promising quantum materials with unique electronic and optical properties for quantum science applications such as quantum computation, sensing, simulation, and communication. While colloidal QDs and QRs can be dispersed in solvents and readily integrated on surfaces and in devices using solution-based assembly techniques, scalable and deterministic arrangement of single and arrayed QDs/QRs on devices with sub-10 nm resolution remains a challenge. We employ robust DNA origami templates to guide the incorporation of colloidal QDs and QRs on device substrates with nanoscale precision.

DNA origami is a powerful platform for the precise assembly and organization of functional nanomaterials, enabling the creation of complex, tailor-made structures with unprecedented accuracy and programmability. While DNA-modified molecules and colloidal metallic nanoparticles are routinely assembled onto DNA origami, QDs and QRs have been challenging to incorporate due to low DNA conjugation efficiency. We have developed an ultrafast dehydration-assisted method to conjugate a dense layer of ssDNA onto QDs/QRs directly from organic solvent to facilitate their precise and stable assembly on DNA origami templates [1]. To arrange QR arrays on the surface, we developed a Surface-Assisted Large-Scale Assembly (SALSA) strategy to fabricate 2D DNA origami lattices tethered by unique crossover interactions directly on a solid substrate [1]. Alignment of the QRs in the 2D lattice was achieved through predefined binding strands linearly arranged on the origamis to unlock polarized light emission along the long axis of the arrayed QRs. To integrate DNA-templated QDs/QRs into chip-based photonic devices, we further employed lithography to guide the deterministic patterning of precisely positioned and oriented individual DNA origami templates on silicon chips. Landing pads of matching size and shape of the DNA origami were first fabricated using electron beam lithography, followed by origami placement through electrostatic interaction-guided self-assembly. QDs and QRs were then assembled onto the origami templates with predefined position and orientation. Our methods offer significant potential for the precise integration of high-quality colloidal QDs and QRs as quantum emitters for integrated quantum photonics.

1. Chen, C., Luo, X., Kaplan, A. E. K., Bawendi, M. G., Macfarlane, R. J., & Bathe, M. (2023). **Science Advances**, 9(32), eadh8508.

QS-ThP-3 ManQala - a Quantum Game with Implications for Quantum State Engineering, ***Thomas A. Searles***, University of Illinois - Chicago

The ability to prepare systems in specific target states through quantum engineering is essential for realizing the new technologies promised by a second quantum revolution. Here, we cast the fundamental problem of state preparation as ManQala, a quantum game inspired by the West African sowing game mancala. Motivated by optimal gameplay in solitaire mancala, where nested nearest-neighbor permutations and actions evolve the state of the game board to its target configuration, ManQala acts as a pre-processing approach for deterministically arranging particles in a quantum control problem. Once pre-processing with ManQala is complete, existing quantum control methods are applied, but now with a reduced search space. We find that ManQala-type strategies match, or outperform, competing approaches in terms of final state variance even in small-scale quantum state engineering problems where we expect the slightest advantage, since the relative reduction in search space is the least. These results suggest that ManQala provides a rich platform for designing control protocols relevant to quantum technologies.

QS-ThP-4 Correlating the Electronic Structure with the Emergence of Magnetism in $PdCoO_2$, ***Jessica McChesney***, Argonne National Laboratory

Long-range ferromagnetism is induced in the nonmagnetic layered oxide $PdCoO_2$ with the implantation of He. This onset of magnetism was found to be reversible with annealing and tied directly with local lattice distortions. In order to correlate the changes in the electronic structure with the onset of magnetic order, we mapped the Fermi surface and performed resonant photoemission to determine the character of the bands as a function of doping.

QS-ThP-5 How Can Quantum-Based Sensors Be Used for "Nist on a Chip" Sustainability Solutions?, ***Jay Hendricks***, NIST-Gaithersburg*; B. Goldstein,* NIST

This poster covers a bit of metrology history of how we got to where we are today and gives a forward-looking vision for the future of measurement science and its important role in our daily lives. The role of NIST as a National Metrology institute (NMI) is briefly described considering the world-wide redefinition of units that occurred on May 20th, 2019. The re-definition of units is now aligned with physical constants of nature and fundamental physics which opens new realization routes with quantum-based sensors and standards. The NIST on a Chip program (NOAC) is briefly introduced in this context.

The technical core is 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. The FLOC will enable the elimination of mercury barometers pressure standards worldwide and the CAVS will be first primary standard for making vacuum measurements below 1.3×10^{-5} Pa. A Sensitive Photonic Thermometer (SPOT) will be introduced, along with other sensing technologies that the NOAC program is currently investigating such as flux, magnetic field, and mass and torque.

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 devices? What will be the role of metrology institutes in the is new ecosystem of metrology and measurement? What will be the NMI role for solutions aimed at sustainability and environment? This posterwill begin to explore these important philosophical questions.

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