## Materials and Processes for Quantum Information, Computing and Science Focus Topic
## Room B231-232 - Session QS+EM+MN+NS-MoM

### High Coherence Qubits for Quantum Computing

**Moderators:** Vivekananda Adiga, IBM, T.J. Watson Research Center, Martina Esposito, Oxford University, UK

8:20am **QS+EM+MN+NS-MoM-1 Measurement of a Two-Level-System Dipole Distribution in a Nanoscale Aluminum Oxide Barrier*, Chih-Chiao Hung*, *N Foroozani, K Osborn,* University of Maryland

Random atomic-sized material defects, identified as two-level systems (TLS), have garnered wide interest because they cause decoherence in superconducting qubits. TLSs often arise in the nonlinear element, the Josephson junction, which is typically made of amorphous aluminum oxide. This material is a clear concern in qubits due to a substantial loss tangent in bulk: large area JJs. However, detail on the dipole moments of individual TLSs is generally lacking but is fundamental to defect-qubit coupling. We have recently developed a method to study individual dipole moments in thin dielectric films with a quantum regime resonator using an electrical bridge of capacitors. We have now extended this technique to a different material, aluminum oxide, using a smaller nanoscale thicknesses and barrier volume. The geometry of the device allows extraction of the individual dipole moments within the central layer of a superconductor-aluminum oxide-superconductor trilayer. This new study also produced a greater statistical sample of TLS dipoles than previous work. Preliminary analysis allows us to extract a dipole moment distribution with a clear mean value. This information on aluminum oxide can be used in the future modeling of qubits and the future characterization of qubit materials.

8:40am **QS+EM+MN+NS-MoM-2 Mapping Quantum Systems to Quantum Computers using Symmetry*, Daniel Gunlycke*, *S Fischer, S Hellberg, S Policastro, S Tafur,* U.S. Naval Research Laboratory

Quantum entanglement is a natural phenomenon in quantum mechanics that has enormous significance in quantum information science, including quantum computing. It enters quantum states in quantum algorithms through the application of multi-qubit quantum logic operations such as the CNOT and Ising gates. While deliberate entanglement adds power and efficiency to algorithms, unintentional entanglement can be undesirable for a variety of reasons. Unintentional entanglement adds complexity, making the outcome of a given algorithm more difficult to understand, as well as more sensitive to errors. Furthermore, it can be an indication that an algorithm has not been optimized. If we could transfer entanglement from our algorithms into the bases that define our systems, then we could potentially reduce our algorithms, including the qubit requirement. Such algorithm reductions will be of outmost importance for resource-limited, noisy intermediate-scale quantum (NISQ) computers.

In this presentation, we will demonstrate how such a reduction could be achieved for the simulation of quantum systems using symmetry. In addition to reducing the needed resources, our quantum computer calculations show a significant improvement in accuracy.

9:00am **QS+EM+MN+NS-MoM-3 History of Superconducting Qubit Coherence and the Current Challenges*, Hanhee Paik*,** IBM T.J. Watson Research Center **INVITED**

Since the first demonstration of a few nanoseconds of coherent oscillations in 1999, a tremendous amount of effort has been put in to improve coherence of superconducting qubits. A modern day superconducting qubits show typically 100 microseconds of coherence times which allowed us to demonstrate a few simple quantum computing applications that led rapid growth of quantum computing industry. To build a full fault-tolerant universal quantum computing system, however, we still need a couple more orders of magnitude improvement in the superconducting qubit coherence, the solution to which, we believe, is in the qubit materials. In this talk, I will review the history of the superconducting qubit coherence research and what we learned about the materials for quantum computing at milli-kelvin temperatures, and I will discuss the current challenges of the coherence studies in the conjunction with the challenges in material science research.

9:40am **QS+EM+MN+NS-MoM-5 Loss and Decoherence Benchmarking of Superconducting Transmon Qubits*, Jonas Bylander*,** Chalmers University of Technology, Sweden **INVITED**

We are engineering a superconducting quantum processor within the Wallenberg Center for Quantum Technology [1] in Sweden and the project OpenSuperQ [2] of the European Union's Flagship on Quantum Technology.

Here we will present our engineering approach for high-coherence superconducting quantum hardware. We have studied the temporal stability of relaxation and dephasing in transmon qubits [3]. Our qubits are made of aluminum on silicon; they have reached average $T_1$ relaxation times of about 70 us. The $T_2^*$ decoherence time, as measured in a Ramsey fringe, is practically relaxation-limited. By collecting statistics during measurements spanning several days, we reveal large fluctuations of qubit lifetimes – the standard deviation of $T_1$ is about 15 us – and find that the cause of fluctuations is parasitic, near-resonant two-level-systems (TLS). Our statistical analysis shows consistency with an interacting-TLS model. Interacting TLS also cause low-frequency capacitance fluctuations, ultimately leading to frequency noise and dephasing of the qubit state. These discoveries are important for creating stable superconducting circuits suitable for high-fidelity quantum gates in quantum computing applications.

[1] www.wacqt.se

[2] www.opensuperq.eu

[3] J. J. Burnett, A. Bengtsson, M. Scigliuzzo, D. Niepce, M. Kudra, P. Delsing, and J. Bylander, "Decoherence benchmarking of superconducting qubits" arXiv:1901.04417

10:40am **QS+EM+MN+NS-MoM-8 Towards PAMBE Grown Nitride Superconductors for Epitaxial Josephson Junctions and Quantum Circuits*, Christopher Richardson*,** *A Alexander, C Weddle,* Laboratory for Physical Sciences*; M Olszta, B Arey,* Pacific Northwest National Laboratory **INVITED**

Low microwave loss superconducting circuit components are a necessity of fabricating high-fidelity superconducting qubits. Accordingly, significant research has focused on making high-quality planar resonators from elemental and nitride superconductors. Josephson junctions are the nonlinear component of superconducting qubits, that also need to be high performance. Interestingly, superconducting qubits all use Josephson junctions fabricated from aluminum and aluminum oxide using the double angle evaporation process. Details of this alternative design will be presented.

Plasma assisted Molecular beam epitaxy (PAMBE) is used to grow niobium titanium nitride alloys ($Nb_xTi_{1-x}N$) and wide bandgap nitride (AlN) superconductors directly on sapphire wafers. This combination of nitride materials provides sufficient degrees of freedom that synthesis of an epitaxial Josephson junction may be possible. Using a structure first approach to design optimization, the structural, surface topology, chemical characteristics, and superconducting critical temperature of these films are used for optimization of the growth conditions before resonators are fabricated and tested.

Growth results of NbTiN and AlN films, bi-layer insulator-superconductor structures and trilayer superconductor-insulator-superconductor structures will be presented along with superconducting properties.

11:20am **QS+EM+MN+NS-MoM-10 Josephson Junction Metrology for Superconducting Quantum Device Design*, Ruichen Zhao*,** *M Bal, J Long, R Lake, X Wu, C Rae McRae, H Ku, H Wang, D Pappas,* National Institute of Standards and Technology (NIST)

Josephson junctions (JJs) are the power horses that drive the development of superconducting quantum technologies in the past decades. The non-linear inductance of JJs turns superconducting circuitry into a high-coherence two-level system that forms the foundation for quantum information processing [1]. They also enable Josephson parametric amplification that significantly improves the measurement of the fragile quantum state of superconducting qubits, mechanical oscillators or spins [2]. Consequently, the characterization of junction inductance becomes essential for the design and fabrication of these superconducting quantum devices.

Here, we present a systematic approach to characterize the micron-size JJs made from a new process. This new recipe extends from our previous work on nanoscale overlapping qubit junctions [1]. First, we collect statistics of the normal-state resistance over 2000 JJs through the room-temperature automated probing test. Second, we use Ambegaokar-baratoff formula to map the normal-state junction resistance into Josephson inductance [3].

Then we extract and investigate the process bias of our JJs. Based on this new information of JJs variation, we proposed a new JJ process which could potentially provide better control over the Junction inductance and therefore, deliver more reliable parameters for the device design.

[1] X. Wu, et al. "Overlap junctions for high coherence superconducting qubits." Applied Physics Letters 111.3: 032602 (2017).

[2] M. Malnou, et al. Optimal operation of a Josephson parametric amplifier for vacuum squeezing. Physical Review Applied, 9(4), 044023 (2018).

[3] V. Ambegaokar, & A. Baratoff, “Tunneling between superconductors.” Physical Review Letters, 10(11), 486 (1963).

11:40am **QS+EM+MN+NS-MoM-11 Superconducting Metamaterial Resonator Spectrum and Interaction with Qubit***, **Haozhi Wang**, S Indrajeet, M Hutchings, M LaHaye, B Plourde,* Syracuse University*; B Taketani, F Wilhelm,* Saarland University

Metamaterial transmission line resonators fabricated from superconducting thin films can be designed to exhibit novel mode spectra like a high density of modes in the same frequency range where superconducting qubits are typically operated. We demonstrate the mode spectrum of a metamaterial resonator made of single layer of Nb and the coupling quality factor of the modes. We also present a series of low-temperature measurements of such a superconducting metamaterial resonator coupled to a flux-tunable transmon qubit. We observe Rabi vacuum crossing when performing transmission measurement of the metamaterial resonator as we tune the qubit frequency through many of the metamaterial resonances and we are able to track the qubit using a separate conventional resonator to read out the qubit state.

## Materials and Processes for Quantum Information, Computing and Science Focus Topic
## Room B231-232 - Session QS+EM+MN+NS+VT-MoA

### Systems and Devices for Quantum Computing

**Moderators:** Jonas Bylander, Chalmers University of Technology, Sweden, Ruichen Zhao, National Institute of Standards and Technology (NIST)

1:40pm **QS+EM+MN+NS+VT-MoA-1 DEMUXYZ Gate Using Single Microwave Drive Line for Multiple Qubits***, **Matteo Mariantoni,*** University of Waterloo, Canada*; C Earnest,* University atof Waterloo, Canada*; J Béjanin,* University of Waterloo, Canada

Superconducting qubits have the potential to lead to large-scale quantum computers with $10^5$ or more qubits in 2D arrays. As the number of qubits increases, finding methods to connect all the necessary control lines to each qubit can become a serious challenge. In this talk, we introduce a new demultiplexed one-qubit gate: DEMUXYZ. This gate makes it possible to decrease the number of microwave control lines from $N^2$ to 1 by allowing multiple qubits to share a single microwave line. The shared line carries a continuous wave (CW) microwave tone, which is initially detuned from the qubits' idle frequency. When a qubit must undergo an arbitrary rotation on the Bloch sphere, the qubit is tuned on resonance with the CW tone and allowed to interact with the drive for the duration required to achieve the desired rotation. The rotation phase is tuned by detuning the qubit frequency away from the drive and idle frequency for the required time length. We demonstrate a first proof of concept for this gate performing experiments on Xmon transmon qubits. We characterize the gate ON/OFF ratio and perform quantum state tomography.

**Funding Acknowledgement:** This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund (CFREF) and the Discovery and Research Tools and Instruments Grant Programs of the Natural Sciences and Engineering Research Council of Canada (NSERC).

2:00pm **QS+EM+MN+NS+VT-MoA-2 Structural and Electronic Characterization of a Novel Si/SiGe Heterostructure for Quantum Computing***, **Thomas McJunkin,** E MacQuarrie, S Neyens, B Thorgrimsson, J Corrigan, J Dodson, D Savage, M Lagally, R Joynt, M Friesen, S Coppersmith, M Eriksson,* University of Wisconsin - Madison

In recent years, silicon-based quantum dots have been shown to be a promising avenue for quantum computing. However, dots formed in silicon quantum wells exhibit a near-degeneracy of the two low-lying valley states. Motivated by a desire to increase the magnitude and tunability of this valley splitting, we report the characterization of a novel Si/SiGe heterostructure grown with a thin layer of SiGe embedded within the Si quantum well, near the top of the well. The Si/SiGe heterostructure is grown via UHV-CVD on a linearly graded SiGe alloy with a final Ge concentration of 29%. STEM measurements reveal the quantum well structure to consist of a ~10 nm Si layer, followed by a thin ~1 nm SiGe layer, and subsequent ~2 nm layer of pure Si. Above this quantum well, a ~35 nm layer of SiGe with 29% Ge is grown to separate the quantum well from the surface. The intent of this ~1 nm layer of SiGe, positioned just below the upper interface of the quantum well, is to modify the valley splitting of electrons in a 2-dimensional electron gas (2DEG) that reside near this interface. By modifying an external vertical electric field, the electron wavefunction can be moved on and off this spike in germanium concentration.

We report electronic measurements of both Hall bars and quantum dot devices that are fabricated on this heterostructure. Shubnikov-de Haas (SdH) and quantum Hall (QH) measurements reveal a peak transport mobility in excess of 100,000 $cm^2/(V s)$ at 6 x $10^{11}$ $cm^{-2}$ carrier density . We report SdH and QH measurements over a wide range of carrier density and magnetic field in the form of a fan diagram. Valley splitting values are measured in the quantum dot device by magnetospectroscopy, in which a few-electron dot transition is measured as the in-plane magnetic field is swept. Measuring at the second, third, and fourth electron transition in the quantum dot, we find valley splittings of 29, 48, and 65 ueV, respectively. To measure tunability of valley splitting, nearby gate voltages are changed to vary the vertical electric field at constant charge occupation. We find that both the lowest lying valley splitting and the valley splitting in the first excited orbital can be tuned over a factor of 2 by means of such changes in gate voltage.

2:20pm **QS+EM+MN+NS+VT-MoA-3 Efficient Quantum Computation using Problem-specific Quantum Hardware and Algorithms***, **Stefan Filipp,*** IBM Research - Zurich, Switzerland **INVITED**

In recent years we have observed a rapid development of quantum technologies for the realization of quantum computers that promise to outperform conventional computers in certain types of problems. This includes problems in optimization, machine learning, finite element calculations, and in the computation of complex molecules. A key requirement to perform computations on current and near-term quantum processors is the design of quantum algorithms with short circuit depth that finish within the coherence time of the qubits. To this end, it is essential to implement a set of quantum gates that are tailored to the problem at hand and that can be directly implemented in hardware. To efficiently compute the ground and excited states of molecular hydrogen we utilize a parametrically driven tunable coupler to realize exchange-type gates that are configurable in amplitude and phase on two fixed-frequency superconducting qubits. Such gates are particularly well suited for quantum chemistry applications because they preserve the number of qubit excitations corresponding to the fixed number of electrons in the molecule. With gate fidelities around 95% we compute the eigenstates within an accuracy of 50 mHartree on average, an good starting point for the simulation of larger molecular systems.

3:00pm **QS+EM+MN+NS+VT-MoA-5 Reconfigurable Magnetic Textures for Quantum Information Applications***, **Alex Matos-Abiague,*** Wayne State University **INVITED**

Spintronic devices such as spin valves have extensively been used for non-volatile memory applications. The magnetic fringe fields generated by spin valves strongly depend on the magnetic state of the device. Thus, an array of electrically switchable spin valves allows for the generation of reconfigurable magnetic textures whose specific form and properties can be controlled on the nanometer scale. When combined with materials with large g-factor, such magnetic textures can have sizable effects not only on the spin but also on the localization, exchange, and transport properties of carriers. We show how the local control of the fringe-field-generated magnetic texture provides a unique tool for creating effective reconfigurable nanostructures and how it can be used for various quantum information applications. In particular, we focus on the use of reconfigurable magnetic textures as a new path to the realization of fault-tolerant topological quantum computing by enabling the generation and manipulation of Majorana bound states (MBSs) in superconductor/semiconductor heterostructures [1-4]. MBSs are emergent quasiparticles that obey non-Abelian statistics and can store quantum information that is immune against smooth local perturbations. Magnetic textures can provide not only synthetic spin-orbit and Zeeman fields -two important ingredients for the creation of MBSs- but also spatial confinement by creating closed domains in the form of effective topological wires. The effective wires can be re-shaped and re-oriented by properly changing the magnetic texture, allowing for the transportation of the MBSs [1,3] and the realization of quantum gates through braiding operations [2]. Other platforms combining the use of reconfigurable magnetic textures and Josephson junctions, as well as the main experimental challenges regarding materials, scalability, and detection are also discussed.

ACKNOWLEDGMENTS: This work is supported by DARPA Grant No.DP18AP900007 and US ONR Grant No. N000141712793

[1] G. L. Fatin, A. Matos-Abiague, B. Scharf, I Žutić, Phys. Rev. Lett. **117**, 077002 (2016).

[2] A. Matos-Abiague, J. Shabani, A. D. Kent, G. L. Fatin, B. Scharf, I. Žutić, Solid State Commun. **262**, 1 (2017).

[3] T. Zhou, N. Mohanta, J. E. Han, A. Matos-Abiague, and I. Žutić, Phys. Rev. B **99**, 134505 (2019).

[4] N. Mohanta, T. Zhou, J. Xu, J. E. Han, A. D. Kent, J. Shabani, I. Žutić, and A. Matos-Abiague, arXiv:1903.07834

4:00pm **QS+EM+MN+NS+VT-MoA-8 Coaxial Multilayer Superconducting Circuits for Quantum Computing***, **Peter Leek,*** University of Oxford, UK **INVITED**

Superconducting circuits are one of the leading candidates for the realization of quantum computers, in particular for near-term applications which may already be reached with circuits consisting of a few hundred qubits, provided they are operated at high fidelity. Until recently, the topology of superconducting circuits has typically been constrained to two dimensions, which becomes difficult to scale as the number of qubits increases and control and measurement wiring is needed for qubits in the middle of large arrays. It is natural to explore new circuit topologies that incorporate wiring in the third dimension to solve this problem. In this talk I will present an overview of an approach that builds on a coaxially-symmetric circuit QED unit cell with out-of-plane wiring [1] that provides a simple route to scaling to grids of many qubits. In this approach, arrays of qubits and resonators can be fabricated on opposing sides of a substrate and capacitively coupled, while control and readout are achieved via off-chip coaxial wires which run perpendicular to the chip plane and are built into a precision micro-machined enclosure that provides a high-quality microwave environment for the circuit.

[1] Rahamim et al., Applied Physics Letters **110**, 222602 (2017)

4:40pm **QS+EM+MN+NS+VT-MoA-10 Josephson Parametric Amplifiers based on Micron Scale Overlap Junctions (O-JPA)***, **Mustafa Bal**, J Long, R Zhao, H Wang,* National Institute of Standards and Technology (NIST)*; C McRae,* National Institute of Standards and Technology (NIST) and University of Colorado Boulder*; R Lake, X Wu, H Ku, D Pappas,* National Institute of Standards and Technology (NIST)

Quantum limited amplifiers have become indispensable tools in superconducting quantum circuits. In recent years, quantum limited amplification has been demonstrated in parametric amplifiers based on high kinetic inductance superconductors as well as Josephson junctions. Previously, we have demonstrated submicron scale overlap Josephson junction fab process for qubits with long coherence times [1]. Here, we extend the overlap junction fab process to micron scale junctions to enable the realization of other superconducting quantum devices such as overlap junction-based Josephson parametric amplifiers (O-JPA). Our fab scheme yield frequency tunable O-JPAs with negligible insertion loss. We readily observe over 25 dB gain. Compared to other competing processes, overlap junction process for micron scale junctions allows the fabrication of O-JPAs with high yield and good device performance at a much lower infrastructure requirements. The fabrication details of overlap junction process as well as the results of O-JPA characterization will be presented. The metrology of overlap Josephson junctions will also be presented in this this symposium [2].

[1] X. Wu, J. L. Long, H. S. Ku, R. E. Lake, M. Bal, and D. P. Pappas, “Overlap junctions for high coherence superconducting qubits”, Appl. Phys. Lett. **111**, 032602 (2017).

[2] R. Zhao *et al*., “Josephson Junction metrology for superconducting quantum device design”, also presented at AVS 66$^{th}$ International Symposium & Exhibition.

5:00pm **QS+EM+MN+NS+VT-MoA-11 Development and Characterization of a Flux-pumped Josephson Parametric Amplifier***, **Martina Esposito**,* University of Oxford, UK

Josephson parametric amplification is a tool of paramount importance in circuit quantum electrodynamics (circuit-QED), especially for the quantum-noise-limited single-shot readout of superconducting qubits. Here we present the development and characterization of a flux-pumped Josephson parametric amplifier (JPA) based on a lumped-element LC resonator, in which the inductance L is composed by a geometric inductance and an array of superconducting quantum interference devices (SQUIDs) [1]. In addition, we show preliminary experiments where the JPA is used as the first stage of amplification for the readout of a superconducting qubit based on a coaxial architecture recently developed in our lab in Oxford [2]. Finally, we will introduce future scientific direction based on using JPAs for generation and control of non-classical states in microwave photons.

[1] M. Esposito et al. EPJ Web of Conferences 198, 00008 (2019)

[2] J. Rahamim et al. Applied Physics Letters 110, 222602 (2017)

## 2D Materials
## Room A226 - Session 2D+EM+MI+MN+NS+QS-TuM
### Novel Quantum Phenomena

**Moderator:** Arend van der Zande, University of Illinois at Urbana Champaign

8:00am **2D+EM+MI+MN+NS+QS-TuM-1 Charge Density-Wave States in Single-Layer Transition-Metal Dichalcogenides***, **Phil King**,* University of St Andrews, UK **INVITED**

Control over materials thickness down to the single-atom scale has emerged as a powerful tuning parameter for manipulating not only the single-particle band structures of solids, but increasingly also their interacting electronic states and phases. A particularly attractive materials system in which to explore this is the transition-metal dichalcogenides, both because of their naturally-layered van der Waals structures as well as the wide variety of materials properties which they are known to host. Yet, how their interacting electronic states and phases evolve when thinned to the single-layer limit remains a key open question in many such systems. Here, we use angle-resolved photoemission to investigate the electronic structure and charge density wave (CDW) phases of monolayer $TiSe_2$, $TiTe_2$, and $VSe_2$. Three-dimensionality is a core feature of the electronic structure of all of these parent compounds, but we show how their CDW phases not only persist, but are strengthened, in the monolayer limit. In $TiSe_2$, we observe an orbital-selective CDW, necessarily without a $k_z$-selectivity in band hybridisation that is of key importance for the bulk instability,[1] while $TiTe_2$ is driven into a charge-ordered phase in the monolayer which is not stable in the bulk at all. In $VSe_2$, we show how the monolayer hosts a much stronger-coupling CDW instability than the bulk, which in turn drives a metal-insulator transition, removing a competing instability to ferromagnetism.[2] Together, these studies point to the delicate balance that can be realized between competing interacting states and phases in monolayer transition-metal dichalcogenides.


*This work was performed in close collaboration with M.D. Watson, A. Rajan, J. Feng, D. Biswas, and colleagues from the Universities of St Andrews, Oxford, Keil, Diamond, Elettra, and SOLEIL.*



[1]Watson *et al.*, Phys. Rev. Lett. 122 (2019) 076404.

[2]Feng *et al.,* Nano Lett. 18 (2018) 4493.


8:40am **2D+EM+MI+MN+NS+QS-TuM-3 Sublattice Symmetry Breaking and Kondo-effect Enhancement in Strained Graphene***, D Zhai,* Ohio University*; K Ingersent,* University of Florida*; S Ulloa, **Nancy Sandler**,* Ohio University

Kondo physics in doped monolayer graphene is predicted to exhibit unusual features due to the linear vanishing of the pristine material's density of states at the Dirac point. Despite several attempts, conclusive experimental observation of the phenomenon remains elusive. One likely obstacle to identification is a very small Kondo temperature scale *TK* in situations where the chemical potential lies near the Dirac point. We propose tailored mechanical deformations of monolayer graphene as a means of revealing unique fingerprints of the Kondo effect. Inhomogeneous strains are known to produce specific alternating changes in the local density of states (LDOS) away from the Dirac point that signal sublattice symmetry-breaking effects. Small LDOS changes can be amplified in an exponential increase or decrease of *TK* for magnetic impurities attached at different locations. We illustrate this behavior in two deformation geometries: a circular "bubble" and a long fold, both described by Gaussian displacement profiles. We calculate the LDOS changes for modest strains and analyze the relevant Anderson impurity model describing a magnetic atom adsorbed in either a "top-site" or a "hollow-site" configuration. Numerical renormalization-group solutions of the impurity model suggest that higher expected *TK* values, combined with distinctive spatial patterns under variation of the point of graphene attachment, make the top-site configuration the more promising for experimental observation of signatures of the Kondo effect. The strong strain sensitivity of *TK* may lift top-site Kondo physics into the range experimentally accessible using local probes such as scanning tunneling microscopy.

9:00am **2D+EM+MI+MN+NS+QS-TuM-4 Indirect Transition and Opposite Circular Polarization of Interlayer Exciton in a MoSe2 WSe2 van der Waals Heterostructure***, **Hsun-Jen Chuang**, A Hanbicki, M Rosenberger, C Hellberg, S Sivaram, K McCreary, I Mazin, B Jonker,* U.S. Naval Research Laboratory

An emerging class of heterostructures involves monolayer semiconductors such as many of the transition metal dichalcogenides (TMDs) which can be combined to form van der Waals heterostructures (vdWHs). One unique new optical property of heterostructure is an interlayer exciton (ILE), a spatially indirect, electron-hole pair with the electron in one TMD layer and the hole in the other. Here, we fabricated MoSe2/WSe2 hetero-bilayer encapsulated in h-BN with the alignment angle close to 60 degree between MoSe2 and WSe2. Followed by the state-of-the-art preparation techniques (Nano-squeegee) to ensure the optimal contact between the TMDs. The Strong ILE emission is observed with the emission energy around 1.35 eV at room temperature and resolve this emission into two distinct peaks (ILE1 and ILE2) separated by 24 meV at zero field at 5 K. Furthermore, we demonstrate that the two emission peaks have *opposite*circular polarizations with up to +20% for the ILE1 and -40% for ILE2 when excited by circularly polarized light. A*b initio* calculations provide an explanation of this unique and potentially useful property and indicate that it is a result of the indirect character of *both* electronictransitions. These peaks are *doubleindirect* excitons. *i.e.*indirect in both real and reciprocal space, split by relativistic effects.


This research was performed while H.-J.C. held an American Society for Engineering Education fellowship and M.R.R and S.V.S held a National Research Council fellowship at NRL. This work was supported by core programs at NRL and the NRL Nanoscience Institute. This work was also supported in part by a grant of computer time from the DoD High Performance Computing Modernization Program at the U.S. Army Research Laboratory Supercomputing Resource Center.


9:20am **2D+EM+MI+MN+NS+QS-TuM-5 Integrating 2D Magnet 1T-$MnSe_2$ with Topological Insulator $Bi_2Se_3$***, **Tiancong Zhu**,* The Ohio State University*; D O'Hara,* University of California, Riverside*; J Repicky, S Yu, M Zhu, B Noesges, T Liu, M Brenner, L Brillson, J Hwang, F Yang, J Gupta, R Kawakami,* The Ohio State University

Integrating two-dimensional(2D) magnet with topological insulator is an exciting topic. Other than the possible proximity induced magnetic ordering inside topological insulator, the 2D magnet/ topological insulator heterostructure can also lead to more efficient spin orbit torque switching, or the formation of magnetic skyrmions. The recent discovery of room temperature ferromagnetic ordering in 2D material MnSe and VSe further brings more potential in such heterostructure systems. In this talk, we report the synthesis and characterization of 2D magnet 1T-MnSe on topological insulator Bi Se . Monolayer of MnSe is grown on Bi Se with molecular beam epitaxy, and subsequently characterized with various techniques, including X-ray diffractometry (XRD), X-ray photoemission spectroscopy (XPS) and scanning tunneling microscopy (STM). STM measurement reveals the co-existence of monolayer a-MnSe(111) and 1T-$MnSe_2$ on $Bi_2Se_3$ surface. By performing spin-polarized STM measurement with Cr tip, we observed directly the magnetic signal from 1T-$MnSe_2$ on $Bi_2Se_3$. The growth of 1T-$MnSe_2$ on $Bi_2Se_3$ further leads to the MBE synthesis of magnetic topological insulator $Bi_2MnSe_4$, which also shows ferromagnetism down to the monolayer limit. The structural and magnetic characterization of the material will also be discussed in this talk.

9:40am **2D+EM+MI+MN+NS+QS-TuM-6 Effect of Exchange-correlation Functional and Structural Constraints on the Transition Temperature of Two- Dimensional Ferroelectrics***, **Shiva P. Poudel**, J Villanova, B Miller, A Pandit, S Barraza-Lopez,* University of Arkansas, Fayetteville

In this presentation, I will discuss two inconsistent models for obtaining the transition temperature ($T_c$) of two-dimensional (2D) ferroelectrics. It will be shown that the inconsistency arises from the choice of exchange-correlation functional and structural constraints [1-4] by obtaining $T_c$ for a SnSe monolayer with PBE and vdW exchange-correlation functional, and with increased constraints. It has been found that vdW functional gives a larger $T_c$ in comparison with PBE functional. Also, the increasing constraint raises $T_c$ as well. Afterward, a complete analysis of the converged unit cell with seven different exchange-correlation functional will be provided. These results represent the most comprehensive theoretical benchmarks for these intriguing 2D ferroelectric materials.


This work was funded by an Early Career Grant from the DOE (Grant No. DE-SC0016139). Calculations were performed on Cori at the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-

AC02-05CH11231 and Arkansas High-Performance Computing Center's *trestles*, which is funded through the multiple National Science Foundation grants and the Arkansas Economic Development Commission.

References:

1. M. Mehboudi et al., Nano Lett. **16**, 1704 (2016).

2. M. Mehboudi, et al., Phys. Rev. Lett. **117**, 246802 (2016).

3. S. Barraza-Lopez, et al., PRB **97**, 024110 (2018).

4. R. Fei, et al., Phys. Rev. Lett. **117**, 097601 (2016).

11:00am **2D+EM+MI+MN+NS+QS-TuM-10 Sign-change Pairing Symmetry in Single Layer FeSe/SrTiO$_3$ Film*, Huimin Zhang,*** West Virginia University*; Z Ge, M Weinert,* University of Wisconsin*; L Li,* West Virginia University

Single layer FeSe film epitaxially grown on SrTiO$_3$(001) substrate has drawn much interest for its novel interfacial effects, which have led to the highest superconducting temperature ($T_C$) to date amongst all Fe-based superconductors. While several paring states, such as sign-persevering $s_{++}$-wave, sign-changing nodeless *d*-wave and $s_{\pm}$-wave have been suggested, the pairing symmetry remains to be experimentally validated. Here we investigate the intrinsic impurity-induced in-gap bound states and quasiparticle interference (QPI) patterns in single layer FeSe/SrTiO$_3$ by scanning tunneling microscopy/spectroscopy. We observed bound states induced by nonmagnetic impurities, which strongly suggests a sign-changing order parameter. Through detailed analysis of the phase-sensitive QPI patterns, we further confirm that the order parameter indeed changes sign within the electron pockets. This identification of a sign change pairing symmetry in single layer FeSe/SrTiO$_3$ presents a critical step towards the understanding of its high $T_c$ superconductivity.

11:20am **2D+EM+MI+MN+NS+QS-TuM-11 High Temperature Superconductivity in Epitaxial Single Layer FeTe$_{1-x}$Se$_x$/STO(001)*, Qiang Zou,*** *Z Ge, C Yan, H Zhang, L Li,* West Virginia University

Single crystal FeTe exhibits a distinct long-range bicollinear antiferromagnetic order that can be suppressed by alloying with Se, where superconductivity emerges at a critical Se concentration of 0.3 with a $T_C$ of 10 K. In this work, we show that this phase transition can be further modulated by reducing the thickness of FeTe$_{1-x}$Se$_x$, downto the single atomic layer limit. High quality single layer FeTe$_{1-x}$Se$_x$ films are grown on SrTiO$_3$(001) substrate by molecular beam epitaxy and characterized by scanning tunneling microscopy/spectroscopy and angle-resolved photoemission spectroscopy. We find the electronic properties are strongly dependent on the Se content. For $x < 0.1$, hole-like bands cross the Fermi level and form a hole-pocket at the Γ point with no states observed around the M point, indicating no superconductivity. With increasing Se content, the top of the valence bands moves away from the Fermi level, accompanied by a decrease in effective mass at the Γ point. For $x > 0.1$, the hole pocket at Γ point moves below the Fermi level, and an electron-pocket emerges at M point where a superconducting gap opens with a $T_C$ of ~50 K. These findings and their implications for the emergence and stabilization of superconductivity in Fe-based superconductors at reduced dimensions will be presented at the meeting.

11:40am **2D+EM+MI+MN+NS+QS-TuM-12 The Observation of Majorana Zero Mode and Conductance Plateau in an Iron-based Superconductor*, Hong-Jun Gao,*** Institute of Physics, Chinese Academy of Sciences, China **INVITED**

Majorana zero-modes (MZMs) are spatially-localized zero-energy fractional quasiparticles with non-Abelian braiding statistics that hold great promise for topological quantum computing. Recently, by using scanning tunneling microscopy/spectroscopy (STM/STS), a new breakthrough of Majorana zero mode (MZM) was achieved in a single material platform of high-$T_c$ iron-based superconductors, FeTe$_{0.55}$Se$_{0.45}$, which combined advantages of simple material, high- $T_c$, and large ratio of $\Delta/E_F$ [1]. A detail STM/STS study of a FeTe$_{0.55}$Se$_{0.45}$ single crystal, also revealed the mechanism of two distinct classes of vortices present in this system, which directly tied with the presence or absence of zero-bias peak [2]. To further investigated the MZM, it is still needed to find a "smoking-gun" type of evidence for the existence of MZM, and a quantized conductance plateau is widely believed to be one of them. Here we report an observation of the Majorana conductance plateau in vortices on the iron superconductor FeTe$_{0.55}$Se$_{0.45}$ surface by using STM/STS [3]. We found that both extrinsic instrumental convoluted broadening and intrinsic quasiparticle poisoning can reduce the conductance plateau value. When extrinsic instrumental broadening is removed by deconvolution, the plateau is found to nearly reach a $2e^2/h$ quantized value. The direct observation of a conductance plateau on a single zero-mode in a vortex strongly supports the existence and protection of MZMs in this iron-based superconductor, which can serve as a single-material platform for Majorana braiding at relatively high temperature.

* In collaboration with, D.F. Wang[1,2], L.Y. Kong[1,2], P. Fan[1,2], H. Chen[1], S.Y. Zhu[1,2], W.Y. Liu[1,2], L. Cao[1,2], Y.J. Sun[1,2], S.X. Du[1,2,3], J. Schneeloch[4], R.D. Zhong[4], G.D. Gu[4], Liang Fu[5], Hong Ding[1,2,3].

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[1] D. F. Wang et al, *Science.***362**, 333 (2008).

[2] L. Y. Kong et al, arXiv:1901.02293 (submitted to *Nature Physics* on November 19, 2018)

[2] S. Y. Zhu et al, arXiv: 1904.06124 (submitted to *Science* on February 15, 2019)

## Materials and Processes for Quantum Information, Computing and Science Focus Topic
## Room B231-232 - Session QS-TuM

## AVS Quantum Science (ALL INVITED SESSION)

**Moderators:** Eray Aydil, New York University, Ivan Petrov, University of Illinois at Urbana-Champaign

8:00am **QS-TuM-1 Quantum Technologies from Cold Atoms to Matter-waves*, Philippe Bouyer,*** CNRS, France **INVITED**

The remarkable success of atom coherent manipulation techniques has motivated competitive research and development in precision metrology as well as quantum simulation.

Our ability to cool down atoms to temperature near absolute zero lead to the production of new state of matter e.g. dilute atomic Bose-Einstein condensates (BEC) and degenerate Fermi gases (DFG) where the single or collective quantum behaviour of the particles takes over their classical properties. At these temperatures, atoms can be described by matter waves which behaviour can help understanding quantum properties of conduction, or with which we can create matter-wave sensors that are sensitive to rotation, acceleration or gravitation.

Quantum transport (eg the conduction of electrons in an imperfect crystal) is today widely investigated by using atoms in controlled potentials that mimic the properties of a solid or a semiconductor. While the ideal case is when no defects exist in the periodic potentials used to reproduce the solid matrix, it is also possible to introduce controlled disordered that will lead to peculiar quantum conduction properties. Semi-classical theories, such as those based on the Boltzmann equation, often fail to fully describe the transport properties and the ultra-cold atoms provide a "quantum simulator" to investigate such properties. These properties extend from Anderson localization, percolation, disorder-driven quantum phase transitions and the corresponding Bose-glass or spin-glass phases.

Matter-wave inertial sensors – accelerometers, gyrometers, gravimeters – use our exquisite control of the matter-wave resulting form cooling atoms near absolute zero. They are today all at the forefront of their respective measurement classes. Atom inertial sensors provide nowadays about the best accelerometers and gravimeters and allow, for instance, to make the most precise monitoring of gravity or to device precise tests of general relativity. The outstanding developments of laser-cooling techniques and related technologies allowed the demonstration of matter-wave interferometers in micro-gravity. Using two atomic species (for instance $^{39}$K and $^{87}$Rb) allows to verify that two massive bodies will undergo the same gravitational acceleration regardless of their mass or composition, allowing a test of the Weak Equivalence Principle (WEP). New concepts of matter-wave interferometry are also currently developed to study sub Hertz variations of the strain tensor of space-time and gravitation, providing a new window of observation for gravitational waves detectors.

I present here some recent advances in theses fields

8:40am **QS-TuM-3 Generating Maximal Entanglement Between Spectrally Distinct Solid-state Emitters**, *D Hurst,* University of Sheffield, UK*; K Joanesarson,* University of Sheffield, UK, Tech. University of Denmark*; J Iles-Smith,* University of Sheffield, UK*; J Mork,* University of Denmark*; **Pieter Kok**,* University of Sheffield, UK **INVITED**

We show how to create maximal entanglement between two spectrally distinct solid-state emitters embedded in a waveguide Mach-Zehnder interferometer. By tailoring the input to the interferometer, we optimise the concurrence of the emitter qubits states and show that a two-photon input state can generate deterministic maximal entanglement even for emitters with significantly different transition energies and line-widths. The optimal frequency is determined by two competing processes: which-path erasure and interaction strength. Smaller spectral overlap can be overcome with higher photon numbers, and quasi-monochromatic photons are optimal for entanglement generation. Our work reveals a rich underlying structure in multi-photon scattering from two non-identical emitters, and provides a new methodology for solid-state entanglement generation, where the requirement for perfectly matched emitters can be relaxed in favour of optical state optimisation.

9:20am **QS-TuM-5 From Quantum Atom Optics to Living Cells with Sculpted Light**, ***Halina Rubinsztein-Dunlop**, T Neely, G Gauthier, T Bell, A Pritchard, K Goddard-Lee, A Stilgo, I Favre-Bulle, S Zhang, T Nieminen, I Lenton,* University of Queensland, Australia **INVITED**

Spatial light modulators (SLM) or Digital Micromirror Devices (DMD) give us a great flexibility in sculpting light. What is means is that we have perfect tools that can be used for production of configurable and flexible confining potentials and utilise them to confine atoms as well as lager scale objects and conduct novel experiments outlining light –matter interaction in these systems. In general, we divide the techniques that are used to sculpt light to those based on time average methods and those utilising SLMs in either Fourier plane or direct imaging plane. A Gaussian beam can be modulated using two-axis acousto-optic modulator (AOM) to create highly configurable time-averaged traps. SLMs in Fourier plane control the phase and /or amplitude of an input Gaussian beam, with the pattern representing the spatial Fourier transform of the desired amplitude pattern. The optical system then focuses this sculpted light pattern to the plane containing the system of interests, performing a Fourier transform and recovering the desired pattern. The optical system then focuses this sculpted light pattern to the plane containing the system of interests, performing a Fourier transform and recovering the desired pattern. DMD can configure the amplitude of an input beam either in the Fourier plane or in a direct imaging configuration. Sculptured light produced using these methods promises high flexibility and an opportunity for trapping and driving systems ranging from studies of quantum thermodynamics using ultra cold atoms to trapping and manipulating nano and micron-size objects or even making measurements *in-vivo* inside a biological cell.

In this talk, I will present techniques and results that open up new avenues for the study of quantum fluids, be it by providing a concise atomtronic model for predicting superfluid transport or expanding the accessible parameters space available to fundamental studies of turbulence. The results from our studies of Onsager vortices will be also presented. The realization of negative temperature vortex distributions, long predicted by Onsager, open up the experimental study of the full phase-diagram of 2D vortex matter.

Finally I will demonstrate how carefully sculpted light can be used in microsystems including microthermodynamics and heat engines at that scale.

11:00am **QS-TuM-10 Spin-helical Particles: An Enabling Platform for Quantum Matter and Quantum Technologies**, ***Yong P. Chen**,* Purdue University **INVITED**

Spin is one of the most fundamental quantum properties of particles. In this talk I will describe our experimental studies of “spin-helical” particles (analogous to neutrinos with spin locked to the momentum, but for electrons and atoms) as a powerful platform to realize novel quantum matter and enable new applications in quantum technologies --- such asquantum information, quantum energy, and even quantum chemistry. In particular, we have demonstrated spin-helical electrons [1,2] on the surface of “topological insulators” (TI) and discovered a “topological spin battery” [3], opening the possibility to electrically induce and readout a nuclear and electronic spin polarization with exceptionally long lifetime --- which we present as a remarkable demonstration of the “topological protection” unique to TI. We further observe unusual behaviors in superconducting Josephson junctions and SQUIDs made out of our TIs [4,5,6], paving the way for using such spin-helical electrons to realize “topological superconductor” proposed to harbor “majorana fermions” that could enable scalable, topologically-protected quantum computing. Time permits, I may also describe an experiment on spin-helical (bosonic) atoms, realized using light-matter interaction to engineer “synthetic” spin orbit coupling and gauge fields on laser-cooled $^{87}$Rb atoms in a Bose-Einstein condensate (BEC). We demonstrate a new “interferometric” approach for quantum control of chemical reactions (in our case photoassociation of two atoms into a molecule) by preparing reactants in spin superpositions [7]. It would be interesting to extend such ideas and explore such "quantum beam" experiments the context of surface chemistry and catalysis for example.

Refs: [1] J.Tian et al. Sci. Rep. 5, 14293 (2015); [2] J. Tian et al., Nature Comm. 10, 1461 (2019); [3] J.Tian et al., Science Advances 3, e1602531 (2017); [4] Luis A. Jauregui et al., APL 112, 093105 (2018); [5] M.Kayyalha et al., PRL 122, 047003 (2019); [6] M.Kayyalha et al., arXiv:1812.00499; [7] D.Blasing et al., PRL 121, 073202 (2018)

## MEMS and NEMS Group
## Room A210 - Session MN+QS-TuA

### Devices for Quantum Information and Quantum Nanomechanics

**Moderators:** Sebastian Hentz, CEA-LETI, France, Matthew Jordan, Sandia National Laboratories

2:20pm **MN+QS-TuA-1 Fabrication Challenges in Quantum Optomechanics*, Simon Groeblacher,*** Delft University of Technology, The Netherlands, Netherlands **INVITED**

Mechanical systems have recently attracted significant attention for their potential use in quantum information processing tasks, for example, as compact quantum memories or as transducers between different types of quantum systems. Recent advances have allowed to demonstrate non-classical behavior of mechanical motion by coupling a micro-fabricated acoustic resonator to single optical photons. These experiments include the heralded generation and on-demand readout of single phononic excitations, as well as entanglement between two mechanical modes.

Here we would like to discuss how we fabricate the optomechanical crystals used in these quantum experiments, which feature engineered mechanical resonances in the Gigahertz regime that can be addressed optically from the conventional telecom band. We will also show some of the challenges that need to be overcome in order to realize useful devices for real-world quantum information processing applications.

3:00pm **MN+QS-TuA-3 Floquet Dynamics and Time Symmetry Breaking in Arrays of Driven Nanoresonators*, Mark Dykman,*** Michigan State University **INVITED**

Periodically driven modes of nanomechnical resonators and electromagnetic cavities allow one to study peculiar features of quantum dynamics related to the discrete time translation symmetry imposed by the driving. For modes with high quality factors, which are typically studied in the experiment, these features become pronounced already for comparatively weak driving, provided it is resonant. Quantum dynamics of driven modes is described in terms of the Floquet states. Generally, if the system is in a Floquet state, its dynamical variables oscillate with the period of the driving. However, the discrete time-translation symmetry can be broken, leading to what is called the time crystal effect. For arrays of coupled vibrational modes, the symmetry breaking can occur both in the coherent and dissipative regimes. In the both regimes the transitions are induced by quantum fluctuations, making them nonequilibrium quantum phase transitions. However, the coherent and dissipative transitions are very different. The structure of the emerging states strongly depends on the disorder in the resonator arrays. We will discuss the transitions for the modes driven parametrically close to twice their eigenfrequency and also for the modes driven close to triple the eigenfrequency. Along with the theory we will discuss the ways of observing the vibrational time crystals in the experiment.

4:20pm **MN+QS-TuA-7 Engineering Quantum Signal Transduction in Atomic Layer 2D Devices*, Philip Feng,*** Case Western Reserve University **INVITED**

An essential theme of the ongoing ‘second quantum revolution’ is to realize human-made structures and devices where ‘quantum phenomena’ can be sustained and harnessed to enable radically new approaches to information processing. These require exquisite creation and scalable fabrication of atom-like devices, design and engineering of new information carriers and transduction schemes. Atomic layer crystals have emerged as attractive enablers for creating atomically thin 2D devices that can support signal transduction and information processing functions in the regime where classical meets quantum. In this presentation, we will report on our latest effort and results on developing novel 2D devices (including nanomechanical and photonic resonators, phononic waveguides, photodetectors, etc.), investigating quantum emitters and coupling effects on relevant 2D device platforms, and engineering both classical and quantum signal transduction schemes in such 2D devices and systems.

5:00pm **MN+QS-TuA-9 Superconducting Resonators as Diagnostics for Qubit Fabrication*, Rupert Lewis,*** Sandia National Laboratories **INVITED**

Quantum bits (qubits) fashioned from superconducting thin films and Josephson junctions require different fabrication approaches than back-end-of-the-line semiconductor fab. This

point is driven home most clearly by the realization that the qubit as an anharmonic singlephoton

microwave resonator. The presence of single photon in the qubit represents a one, the

absence represents a zero, thus if the photon is lost, the quantum state is also lost. In

consequence, fabricators of qubits go to extremes to provide low microwave loss environments

for their qubits. Planar microwave resonators—of the multiphoton variety—are an invaluable

diagnostic tool for assessing loss mechanisms in qubit fabrication and the quality of processes

used. This presentation will give a general overview of superconducting qubits and fabrication

techniques and how microwave resonators improve qubits.

Supported by the Laboratory Directed Research and Development program at Sandia National

Laboratories, a multi-mission laboratory managed and operated by National Technology and

Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International,

Inc., for the U.S. Department of Energy's National Nuclear Security Administration under

contract DE-NA-0003525.

5:40pm **MN+QS-TuA-11 Surface Ion Trap Device Fabrication for Experiments in Quantum Information Science*, Matthew Blain,*** Sandia National Laboratories **INVITED**

Radio-frequency (rf) surface ion traps offer important advantages for realizing precise control of the spatial positioning, as well as motional and electronic states, of trapped ions. The control of ions provided by micro-fabricating planar trap electrodes on a silicon device surface has allowed ion trapping to be at the forefront of experiments in quantum sensing, simulation, and information processing. Engineered surface traps offer the ability to extend the performance of their macroscopic equivalents and can even allow new concepts to be explored in both classical and quantum trapped-ion physics and chemistry. T he ability to fabricate complex and arbitrarily arranged 2-D and 2.5-D trap electrode geometries is critical for numerous trapped ion quantum information science experiments. Surface electrode ion traps [1] have enabled the Kielpinski ion trap CCD (charge coupled device) architecture [2], whereby ions can be shuttled between linear trapping regions via junctions, as well as trap designs, for example triangles [3] or rings [4], optimized for different experimental objectives. The ability to design and fabricate precision through-chip holes for ion loading and photon collection/delivery and to arbitrarily shape trap chips for increased optical access to ions is also critical for rendering a highly evolved ion trap chip technology. As well, micro ion trap chip technologies are beginning to integrate passive and active electronic and photonic capabilities for enhanced performance, including trench capacitors, optical waveguides, and avalanche photodiodes. Aspects of the “micro-systems” approach to the design and integration of surface electrode ion trap devices will be presented.

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

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[2] D Kielpinski, *et al.*, *Nature*, 709, 417(2002)

[3] M Mielenz, *et al.*, *Nature Communications*, 7 (2016) 11839

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## Materials and Processes for Quantum Information, Computing and Science Focus Topic
## Room B231-232 - Session QS+2D+EM+MN+NS-TuA

### Materials for Quantum Sciences

**Moderators:** Matthew R. Rosenberger, U.S. Naval Research Laboratory, Robert Walko, The Ohio State University

2:20pm **QS+2D+EM+MN+NS-TuA-1 Electrically Detected Electron Nuclear Double Resonance Study of Defects in 4H-SiC Bipolar Junction Transistors***, **Ryan Waskiewicz**, B Manning, D McCrory, P Lenahan,* Pennsylvania State University

There is growing interest in the possibilities of SiC in spin-based quantum computation. The development of such spin-based quantum computation will require a fundamental understanding of spin physics of paramagnetic defects in SiC including both electron and nuclear paramagnetism. We utilize electrically detected magnetic resonance (EDMR) detection through spin dependent recombination (SDR). In this study we demonstrate relatively high signal to noise electron nuclear double resonance (ENDOR) in a single fully processed SiC pn junction at room temperature. The electrically detected ENDOR (EDENDOR) involves nitrogen nuclei in close proximity to deep level centers within the depletion region of the pn junction; the deep levels are almost certainly silicon vacancies.

We believe these observations are of importance for at least two reasons: (1) they demonstrate that the enormous analytical power of ENDOR can be extended to the study of problems in conventional solid-state electronics and (2) the results demonstrate a way to directly monitor small numbers of nuclear spins through the measure of electronic currents.

In our EDMR measurements, a slowly varying magnetic field and an oscillating microwave frequency magnetic field are applied to the sample inside a microwave cavity. As in conventional EPR, energy is absorbed by paramagnetic sites when the resonance condition is met. For a simple case, this resonance condition is $h\nu=g\mu_B B\pm\Sigma m_i A_i$, where h is Planck's constant, g is an orientation dependent number typically expressed in a g-tensor, $\mu_B$is the Bohr magneton, B is the magnetic field, $m_i$is the spin quantum number of the $i^{th}$ nucleus, and $A_i$ is the hyperfine interaction of the $i^{th}$ magnetic nucleus. In EDMR, the EPR response is detected through a change in device current, in our case due to SDR.

The devices in this study are 4H-SiC BJTs. The EDMR response obtained on these BJTs is very similar to an EDMR spectrum that has been linked to a silicon vacancy in 4H-SiC MOSFETs. To perform the EDENDOR measurement, the magnetic field is held constant and an NMR frequency sweep is applied to the device. The device current is measured and a large response is measured at what is unambiguously the nuclear frequency of nitrogen. These results demonstrate the analytical power of the EDENDOR measurement, measuring nitrogen in the vicinity of the silicon vacancy defect centers that are measured with EDMR.

This work was supported by the Air Force Office of Scientific Research under award number NO. FA9550-17-1-0242.

2:40pm **QS+2D+EM+MN+NS-TuA-2 Scanning Tunneling Microscopy Studies of Er Adatoms on GaAs (110)***, **Rebekah Smith**, A Benjamin, J Gupta,* The Ohio State University

Rare earth dopants in III-V semiconductors are of interest as high quality optical sources due to the preservation of sharp intra-*f*-shell transitions. The long optical coherence lifetime and narrow energy width of these transitions, at 1.54 um, make them a candidate for quantum communication. Here we investigate Er interactions with host GaAs (110) surface with atomic resolution using STM. Er atoms were deposited via electron beam evaporation onto the GaAs surface at 5 K. We find three different $Er_{ad}$ configurations with varying abundance upon deposition, each with a different surface site location. All three configurations exhibit long-range depressions in STM topographic images, attributed to band bending associated with a positive adatom charge state. Individual Er adatoms can be switched between these states by applying a positive voltage pulse with the STM tip. Tunneling spectroscopy on Er adsorbed at the interstitial sites reveals prominent states within the GaAs bandgap, but no evidence of sharp *f*-shell transitions inferred from bulk optical studies. We also form substitutional $Er_{Ga}$ by applying a larger positive voltage pulse. Substitutional Er appears neutral, which we attribute to it being isoelectronic with Ga. This work acknowledges funding from the DOE (DE-SC0016379).

3:00pm **QS+2D+EM+MN+NS-TuA-3 Defect-based Quantum Systems in Hexagonal Boron Nitride***, **Trong Toan Tran**,* University of Technology Sydney, Australia **INVITED**

Engineering solid state quantum systems is amongst grand challenges in realizing integrated quantum photonic circuitry. While several 3D systems (such as diamond, silicon carbide, zinc oxide) have been thoroughly studied, solid state emitters in two dimensional (2D) materials are still in their infancy. In this talk I will introduce hexagonal boron nitride (hBN) as a promising layered material that hosts ultra bright quantum emitters. I will present several avenues to engineer these emitters in large area hBN multilayers and monolayers using chemical vapour deposition techniques. I will then show unique tuning expeirments and promising results for controlling the emission wavelength of these quantum emitters. At the second part of my talk, I will discuss promising avenues to integrate the emitters with plasmonic and photonic cavities to achieve improved collection efficiency and Purcell enhancement. These are fundamental experiments to realize integrated quantum photonics with 2D materials. I will summarize by outlning challenges and promising directions in the field of quantum emitters and nanophotonics with 2D materials and other wide band gap materials.

4:20pm **QS+2D+EM+MN+NS-TuA-7 Specific Placement of $V_{Si}$ in 4H-SiC for Quantum Technologies using $Li^+$ Implantation***, S Pavunny,* ***Rachael L. Myers-Ward****, D Gaskill,* U.S. Naval Research Laboratory*; E Bielejec,* Sandia National Laboratories*; H Banks, A Yeats,* U.S. Naval Research Laboratory*; M DeJarld,* Raytheon*; S Carter,* U.S. Naval Research Laboratory

Silicon carbide has been a material of interest in the quantum technology field for future applications in communication and sensing due in part to the long spin (S = 3/2) coherent lifetime of the Si vacancies ($V_{Si}$). Additional benefits to using SiC for quantum technologies is wafer scalability and fabrication capability using standard processing techniques, making it a favorable material. To improve emission rates of photoluminescence from the vacancies, exact placement of the $V_{Si}$ within microcavities is necessary. Here we show implanted $Li^+$ into Si-face, 4H-SiC homoepitaxy creates $V_{Si}$ in desired locations. The epitaxial material had no measurable $V_{Si}$ prior to $Li^+$ implantation. The dose of 100 keV $L^{i+}$ ranged from $10^{12}$ – $10^{15}$ $cm^{-2}$ and was directed using a maskless focused ion beam technique with a positional accuracy of ~25 nm. The arrays were characterized with high-resolution scanning confocal fluorescence microscopy. Using a 745 nm excitation source, the photoluminescence ranging from 860 – 975 nm produced the characteristic V1', V1 and V2 lines, with the V1' zero-phonon line being consistent for all measurements. In addition, the V1' intensity showed a linear dependence with implantation dose. Moreover, near single photon emission is obtained from $V_{Si}$ at the lowest doses.

Research at NRL is supported by the Office of Naval Research. Ion implantation was performed at Sandia National Laboratories through the Center for Integrated Nanotechnologies, an Office of Science facility operated for the DOE (contract DE-NA-0003525) by Sandia Corporation, a Honeywell subsidiary.

4:40pm **QS+2D+EM+MN+NS-TuA-8 Silicon Vacancy Point Defect in High-quality Nanobeam Photonic Crystal Cavities in 4H Silicon Carbide***, **Mena Gadalla**, X Zhang, A Greenspon,* Harvard University*; D Bracher,* Harvard GSAS*; R Defo, E Hu,* Harvard University

Silicon carbide (SiC) has recently found promise and applications in the quantum world, because of various fluorescent point defects that serve as an intriguing platform for solid-state quantum information and quantum sensing technologies. One such native point defect is the negatively charged silicon vacancy ($V_{Si}^-$)in the 4H polytype of SiC. This color center can occupy two inequivalent lattice sites, resulting in two distinct zero-phonon-lines (ZPL) at 862nm and 916nm. $V_{Si}^-$ possesses good spin coherence properties, with spin states that can be initialized and read out optically. Unfortunately, low branching ratio is a characteristic of the $V_{Si}^-$ spectrum where a small fraction of the total emission is coupled into the ZPL and the rest is emitted into the phonon sideband. This low emission fraction limits the ability to employ $V_{Si}^-$ in various quantum information schemes. To increase the fraction of light emitted into the ZPL and increase the defect emission rate, we fabricated high-quality factor nanophotonic crystal cavities designed to match the ZPL frequency. Through tuning of the cavity into resonance with the ZPLs, we have demonstrated a 75-fold Purcell enhancement at 4K. This talk will describe the fabrication process for 1D nanobeam photonic crystal cavities, leading to quality factors in excess of $10^4$. The highest cavity-defect interactions depend on resonance in frequency and high spatial overlap of the defect with the maximum electric field within the cavity. Using the cavity as a "nanoscope", revealing defect position, we used laser irradiation annealing at varying times and different laser frequencies to infer the diffusive motion of defects within the cavity. We showed that a systematic and controlled laser annealing can increase the ZPL of the implanted cavity mode by a factor of 4.

5:00pm **QS+2D+EM+MN+NS-TuA-9 Tailoring the Heterogeneities in 2D Materials by Controlled Synthesis and Processing***, **Kai Xiao**, X Li, K Wang, A Oyedele, M Yoon, S Xia, M Mahjouri-Samani, C Rouleau, A Puretzky, L Liang, R Unocic, D Geohegan,* Oak Ridge National Laboratory

Two-dimensional (2D) materials are intrinsically heterogeneous, thereforecontrolling defects, understanding the impact of boundaries and interfaces and developing means to exploit these heterogeneities is a transformative opportunity that could underpin future technologies and energy applications. In this talk, I will discuss the fundamental understanding of the roles of heterogeneities including defects, dopants, edges, strain, and phases in 2D materials on their optoelectronic properties. Through isoelectronic doping in monolayer of $MoSe_2$, the Se vacancies are effectively suppressed and photoluminescence is significantly enhanced. In addition, we demonstrate the non-equilibrium, bottom-up growth approach not only can tailor the defect density far beyond intrinsic levels in monolayers of 2D $MoSe_{2-x}$ but also create new antisite defects in monolayers of $WS_2$during the synthesis. The build-in localized strain in 2D crystals directly grown on patterned curved surface can tune the bandgap of 2D crystals for possible quantum emitting applications. The bottom up synthesis of 2D materials discussed here provides excellent control over the heterogeneity in 2D materials, which can modulate the optical and electrical properties in 2D materials and their heterostructures for ultra-thin and flexible electronics.

**Acknowledgment:** Synthesis science was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division and characterizations were performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

5:20pm **QS+2D+EM+MN+NS-TuA-10 Epitaxial Al Films for Plasmonic and Quantum Computing Applications***, **Ka Ming Law**, S Budhathoki, S Ranjit, F Martin, A Hauser,* The University of Alabama

Superconducting resonators are important for application in quantum computing but require high quality factors. Much work has been done on superconducting resonators fabricated from aluminum thin films on sapphire, and superconducting Josephson tunnel junctions made from aluminum are used as the basis for quantum bit designs. In addition, epitaxial aluminum films has attracted attention in plasmonics due to their superior performance in the UV regime compared to Au and Ag, and their compatibility with current CMOS technology. Sapphire substrates are chemically stable and have low lattice mismatch with aluminum, allowing higher film quality without the need for elaborate substrate preparation and time-consuming growth procedures.

Epitaxial aluminum films were successfully grown by off-axis magnetron sputtering on c-plane sapphire. This study assessed the effects of varying both substrate preparation conditions and growth and prebake temperatures on crystallinity and smoothness. X-ray diffraction and reflectivity measurements demonstrate superior crystallinity and surface smoothness for films grown at 200℃ in15mTorr Ar. An additional substrate preparation procedure which involves 1) a modified RCA procedure and 2) prebake in oxygen environment is shown by atomic force microscopy to be highly effective in reducing void density and depth.

5:40pm **QS+2D+EM+MN+NS-TuA-11 Minimizing Coulomb Oscillation Linewidth on Silicon Quantum Dots***, **Yanxue Hong**, A Ramanayaka, M Stewart, Jr., X Wang, R Kashid, P Namboodiri, R Silver, J Pomeroy,* National Institute of Standards and Technology (NIST)

In quantum science research, both cryogenic temperatures and low measurement noise are required for high fidelity. For silicon quantum dot devices, an increase in either one causes broadening of Coulomb blockade peaks, which is usually referred to as a high electron temperature. Here we report on temperature-dependent (T-dependent) conductance measurements and evaluation of effective electron temperature ($T_{eff}$) using an STM-patterned atom-scale silicon single-electron transistor (SET). Measurements are made in various cryogenic systems over temperatures varying from 10 mK to 25 K. The effective electron temperature is extracted by fitting the experimental data using a theoretical model. We initially find that the measured peak width has a linear dependence on the bath temperature above 1 K and saturates below 1 K. In addition, a considerable mismatch (> 2 K) between the lattice (thermometer) temperature and the carrier temperature ($T_{eff}$) is observed. Therefore, the Coulomb resonance is not only thermally broadened by $T_{eff}$ but also broadened by other T-independent sources such as gate noise, triboelectric noise, etc. We study the origins of the saturation at low temperature regime and analyze factors inducing high $T_{eff}$. We report on progress to reduce the noise and reach an effective temperature of < 300 mK. Since our silicon SETs have high charging energies and large energy level spacings, we also seek to measure the transition from classical (multilevel) regime to quantum (single-level) regime by manipulating the bath temperature.

6:00pm **QS+2D+EM+MN+NS-TuA-12 Micro-magnetic Simulations of Correlated Switching in Touching Nano-magnetic Elements***, **Tejumade Durowade**, V Metlushko,* University of Illinois at Chicago

Nanomagnets hold significant potential for use as building blocks for room temperature quantum computers. Bistability based on stable ground magnetization states means power dissipation can be extremely low and their small size allows magnetization to be maintained for a long period time [1]. With packing density on the order of $10^{10}$ /cm$^2$ and switching frequency in the terahertz range, nanomagnets are a promising replacement for current state of art metal oxide semiconductor processes that are already at the limits of continued scaling. In this work, we present the results of simulations of touching nanomagnetic disks that can be used for room operable quantum computing. Like gears in a mechanical system, the chirality of the magnetization in each disk is determined through interaction with its neighbors. These simulations offer insight into the switching dynamics within the disks as current experimental techniques lack the combined temporal and spatial resolution needed to observe the formation and annihilation of the magnetic domains that facilitate the switching process. The switching of touching symmetric disks can be achieved at zero applied field as the disks settle into a remanent vortex state, meaning minimal energy loss during the process. Due to the quantum exchange force, at the point of contact between disks, the magnetization vectors rotate in the same direction giving rise to opposite chiralities in the disks. Since logic states can be represented using the chirality of the in-plane magnetization, configurations of touching disks can potentially be used to implement basic or complex logic functions. Maintaining coherence of opposite chirality in chains of disks was achieved with the introduction of a biasing element to eliminate the bidirectionality of interaction between disks.

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## 2D Materials
## Room A226 - Session 2D+EM+MI+MN+NS+QS-WeM

### Novel 2D Materials

**Moderator:** Phil King, University of St Andrews

8:00am **2D+EM+MI+MN+NS+QS-WeM-1 A Safari Through Thousands of Layered Materials Guided by Data Science Techniques***, **Evan Reed**, G Cheon,* Stanford University **INVITED**

We have utilized data mining approaches to elucidate over 1000 2D materials and several hundred 3D materials consisting of van der Waals bonded 1D subcomponents, or molecular wires. We find that hundreds of these 2D materials have the potential to exhibit observable piezoelectric effects, representing a new class of piezoelectrics. A further class of layered materials consists of naturally occurring vertical hetero structures, i.e. . bulk crystals that consist of stacks of chemically dissimilar van der Waals bonded layers like a 2-D super lattice. We further combine this data set with physics-based machine learning to discover the chemical composition of an additional 1000 materials that are likely to exhibit layered and two-dimensional phases but have yet to be synthesized. This includes two materials our calculations indicate can exist in distinct structures with different band gaps, expanding the short list of two-dimensional phase change materials. We find our model performs five times better than practitioners in the field at identifying layered materials and is comparable or better than professional solid-state chemists. Finally, we find that semi-supervised learning can offer benefits for materials design where labels for some of the materials are unknown.

8:40am **2D+EM+MI+MN+NS+QS-WeM-3 2D Ferroelectric Semiconductor α-$In_2Se_3$ for Non-Volatile Memory Applications***, M Si, **Peide Ye**,* Purdue University

α-$In_2Se_3$ is a novel two-dimensional (2D) ferroelectric semiconductor. It has a bandgap of ~1.39 eV, room temperature ferroelectricity, the ability to maintain ferroelectricity down to a few atomic layers and the feasibility for large-area growth. Based on the ferroelectric and semiconducting nature of the material, a ferroelectric semiconductor field-effect transistor (FeS-FET) was proposed and experimentally demonstrated [1]. In the FeS-FET, a ferroelectric semiconductor is employed as the channel material while the gate insulator is the dielectric. The two non-volatile polarization states in FeS-FETs exist in the ferroelectric semiconductor channel. Therefore, a high quality amorphous gate insulator can be used instead of the common polycrystalline ferroelectric insulator for Fe-FETs. The fabricated FeS-FETs exhibit high performance with a large memory window, a high on/off ratio over $10^8$, a maximum on-current of 862 µA/µm, low supply voltage with scaled gate insulator and the potential to exceed the existing Fe-FETs for non-volatile memory applications.

[1] M. Si, S. Gao, G. Qiu, J. Qin, Y. Duan, J. Jian, H. Wang, W. Wu, and P. D. Ye, "A Ferroelectric Semiconductor Field-Effect Transistor,", arXiv:1812.02933.

9:00am **2D+EM+MI+MN+NS+QS-WeM-4 *Ab initio* Informed Theory of Axis-dependent Conduction Polarity in Goniopolar Materials***, **Yaxian Wang**, B He, M Arguilla, N Cultrara, M Scudder, J Goldberger, J Heremans, W Windl,* The Ohio State University

$NaSn_2As_2$ has recently been synthesized and was found to be an exfoliatable van der Waals Zintl phase, opening new opportunities for electronic design on the few-atom-thick scale. Although the band structure may suggest a range of metal to semi-metal, it shows strong anisotropy especially in its "polarity", characterized by its dominant carrier type, which strongly affects its electronic and thermal properties. We used DFT calculations to investigate bandstructure and Fermi surface. In addition, we employed BoltzTraP code to calculate the transport behavior in in/cross-plane directions, predicting strongly anisotropic carrier transport and directionally dependent polarity –"goniopolarity" – in this layered material. It is confirmed by experimental thermopower measurements. We show from simulations on a model band structure the Fermi surface geometry origin in a single-band toy model, and we utilize the bandwidth concept from a tight-binding model to give an insight of real space orbital contributions and nature of the bonding states in this layered crystal. Based on that, additional candidate materials for goniopolarity can be proposed, and the design space for goniopolar materials in general will be defined.

9:20am **2D+EM+MI+MN+NS+QS-WeM-5 In-Plane Mechanical Properties and Strain Engineering of 2D Hybrid Organic-Inorganic Perovskites***, **Qing Tu**, I Spanopoulos, S Hao, C Wolverton, M Kanatzidis, G Shekhawat, V Dravid,* Northwestern University

Two-dimensional (2D) hybrid organic-inorganic perovskites (HOIPs) are new members of the 2D materials family with wide tunability, highly dynamic structural features and excellent physical properties. Mechanical strain is inevitable in 2D-HOIP-based applications due to materials processing, thermal expansion and substrate deformation. Understanding the mechanical properties and strain engineering of such functional materials are both fundamentally and practically important to achieve high performance and mechanically stable (flexible) devices. Here the in-plane mechanical properties and the impact of in-plane uniaxial tensile strain on the electronic properties of 2D lead iodide perovskites with a general formula $(CH_3(CH_2)_3NH_3)_2(CH_3\text{-}NH_3)_{n-1}Pb_nI_{3n+1}$ were reported for the first time. The in-plane Young's modulus and breaking strength of ultrathin 2D HOIP flakes were measured by AFM-based nanoindentation of suspended 2D HOIP membranes.[1] The in-plane Young's moduli of 2D HOIPs are smaller than that of conventional covalently bonded 2D materials like graphene and $MoS_2$ due to the much more deformable $[PbI_6]^{4-}$ octahedra structure. Both the Young's modulus and breaking strength first decrease and then plateau as the thickness of 2D HOIP flake increases from monolayer to 4 layers, which is attributed to interlayer slippage during deformation. Ultrathin 2D HOIPs exhibit outstanding breaking strength/Young's Modulus ratio compared to many other widely used engineering materials and polymeric flexible substrates, which renders them suitable for application into flexible electronic devices. Furthermore, the uniaxial tensile strain was found to increase the band gap of 2D HOIPs.[2] Such strain effect on the band gap of 2D HOIPs is fully reversible and depends on the structural unit of the materials. For2D HOIP with n = 5, the strain response of the band gap can be as high as 13.3 meV/%. First-principles simulations show that the strain response of the band gap arises from the rotation of the inorganic $[PbI_6]^{4-}$ octahedra and the consequential Pb-I bond stretching and increase of Pb-I-Pb angle. The observed band gap–strain relationship can be harnessed to map the local mechanical strain in 2D HOIP-based devices and allow 2D HOIPs for sensing applications.

**References**

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[2]. Tu Q, Spanopoulos I, Hao S, Wolverton C, Kanatzidis MG, Shekhawat GS, et al. Probing Strain-Induced Band Gap Modulation in 2D Hybrid Organic–Inorganic Perovskites. ACS Energy Letters. 2019;4(3):796-802.

9:40am **2D+EM+MI+MN+NS+QS-WeM-6 Collective Electronic States of Epitaxial Monolayer 1T-$NbSe_2$***, **Zhuozhi Ge**,* University of Wisconsin*; H Zhang, L Liu, C Yan,* West Virginia University*; M Weinert,* University of Wisconsin*; L Li,* West Virginia University

At the single layer limit, transition metal dichalcogenides (TMDs) can adopt two different structural variants depending on the anionic environment around the metal ions: the anions are arranged in trigonal prismatic fashion in the 1H polymorph, whereas in 1T the arrangement is octahedral. While bulk 1T $NbSe_2$ doesn't exist in nature, here we show that single layer 1T $NbSe_2$ polymorph can be grown by molecular beam epitaxy on epitaxial graphene/SiC(0001) substrates. A (Ö13xÖ13) Star-of-David charge density waves is observed by *in situ* scanning tunnelling microscopy, which persists above room temperature. A gap of 0.50 eV is further observed by tunnelling spectroscopy and angle resolved photoemission spectroscopy, indicating that this monolayer 1T phase of $NbSe_2$ is also a Mott insulator, similar to that of bulk 1T $TaS_2$. Our findings indicate that the presence of epitaxial constraints can generate structural configurations that are prohibited in fully-bonded TMD crystals. These findings and their implication on the collective electronic states of single layer 1T-$NbSe_2$ will be discussed at the meeting.

11:00am **2D+EM+MI+MN+NS+QS-WeM-10 Magnetic Interfaces of MnSe2 Monolayer***, **Tomas Rojas**, S Ulloa,* Ohio University

Until recently, 2D magnetism was thought to occur together with defects or doping on different substrates. This situation changed drastically, as intrinsic Cr-based ferromagnetic monolayer materials were discovered, namely CrI3 and Cr2Ge2Te6. A different material, MnSe2, was predicted as stable ferromagnetic monolayer by first-principles calculations, and it has been successfully grown on several substrates. In this study, the authors confirm the intrinsic ferromagnetism of the monolayer, while for thicker samples they report an interface of the MnSe2 monolayer with bulk α-MnSe(111). This phase of the material is non-magnetic, and yet the observed magnetic moments are of up to twice the value of those in the monolayer alone. In this work, we present a detailed analysis of the interactions at this interface between the two phases, using the Heyd-Scuseria-Ernzerhof hybrid functional. We have studied the effects on the electronic and magnetic structure of both phases of the material, and the dependence on the sample thickness. We study the role that strain plays at the interface, and how it affects the magnetic moments of the structure.

Supported by NSF-DMR 1508325, and Ohio Supercomputer Center .

11:20am **2D+EM+MI+MN+NS+QS-WeM-11 Orbital Design of Topological Insulators from Two-dimensional Semiconductors***, **Shixuan Du,*** Institute of Physics, Chinese Academy of Sciences, China

Two-dimensional (2D) materials have attracted much recent attention because they exhibit various distinct intrinsic properties/functionalities, which are, however, usually not interchangeable. Interestingly, here we propose a generic approach to convert 2D semiconductors, which are amply abundant, to 2D topological insulators (TIs), which are less available, via selective atomic adsorption and strain engineering. The approach is underlined by an orbital design principle that involves introducing an extrinsic -orbital state into the intrinsic -bands of a 2D semiconductor, so as to induce - band inversion for a TI phase, as demonstrated by tight-binding model analyses. Remarkably, based on first-principles calculations, we apply this approach to convert the semiconducting monolayer CuS and CuTe into a TI by adsorbing Na and K respectively with a proper -level energy, and CuSe into a TI by adsorbing a mixture of Na and K with a tuned -level energy or by adsorbing either Na or K on a strained CuSe with a tuned -level valence band edge. Our findings open a new door to the discovery of TIs by a predictive materials design, beyond finding a preexisting 2D TI.

This work is in collaboration with Lei Gao and Jia-Tao Sun from IoP-CAS, Gurjyot Sethi and Feng Liu from University of Utah, Yu-Yang Zhang from UCAS.

11:40am **2D+EM+MI+MN+NS+QS-WeM-12 Rotationally Controlled van der Waals Heterostructures of 2D Materials***, **Emanuel Tutuc**, K Kim, G Burg, H Movva,* The University of Texas at Austin **INVITED**

Heterostructures of atomic layers such as graphene, hexagonal boron-nitride, and transition metal dichalcogenides (TMDs) can serve as testbed for novel quantum phenomena in two-dimensions, and potential device applications. A key ingredient that can add a new dimension to the atomic layer heterostructures palette is the rotational control, and alignment of different two-dimensional (2D) layers. We review here an experimental technique that enables rotationally controlled heterostructures with accurate alignment of the individual layer crystal axes [1]. We illustrate the applicability of this technique to the rotationally aligned double layers of graphene [2], or TMDs [3] separated by a tunnel barrier which display resonant, energy- and momentum-conserving tunneling in vertical transport, consistent with theoretical expectations. When two 2D layers are overlaid with a relative twist, the resulting heterostructure shows a new type of periodicity associated with the moiré superlattice, which are only beginning to be systematically investigated as platform for strongly correlated electron physics. We discuss the electron transport in tunable moiré patterns realized in twisted bilayer [4], and double bilayer graphene heterostructures.

Work done in collaboration with S. K. Banerjee, L. F, Register, B. J. LeRoy, A. H. MacDonald, T. Taniguchi, and K. Watanabe.

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## Materials and Processes for Quantum Information, Computing and Science Focus Topic
## Room B231-232 - Session QS+2D+EM+MN+NS+VT-WeM

### Material Systems and Applications for Quantum Sciences

**Moderators:** Mena Gadalla, Harvard University, Kai Xiao, Oak Ridge National Laboratory

8:00am **QS+2D+EM+MN+NS+VT-WeM-1 Quantum Information at the Molecular Foundry - An Overview of New Toolsets for QIS Research***, **Adam Schwartzberg**, S Cabrini, D Ogletree, A Weber-Bargioni,* Lawrence Berkeley National Laboratory (LBNL)

The fundamental unit of quantum computation and sensing is the qubit, and many physical systems have been investigated for practical realization. These include superconducting Josephson junction circuits, color centers, and isolated cold atoms or ions. Superconducting qubit circuits (SCQBs) being one of the most promising avenues to quantum computation. However, there are limitations to their practical application due to noise sources which shorten their functional lifetime.

In this talk I will introduce a suite of integrated, high-fidelity fabrication instrumentation that will allow new communities of users to investigate the fundamental limits of state-of-the-art quantum systems at the Molecular Foundry. We will enable users to understand existing systems and design new ones by creating a quantum fabrication toolset for directed growth of conventional and novel materials, advanced lithography and pattern transfer paired with in- and ex-situ surface characterization.

Three key QIS fabrication capabilities at the Molecular Foundry:

A robotic fabrication cluster system with materials deposition, including atomic layer and physical vapor depositions, plasma etching, and analytical characterization instrumentation, all automated by and contained within a vacuum sample handling robot.

A high resolution electron beam writing system will allow quantum device patterning with complete flexibility in feature shape, density and size, enabling nanoscale feature control.

A low temperature transport measurement system will allow for the investigation of novel materials for superconductors and dielectrics and “close the loop” between design and fabrication, proxy measurements such as interface characterization, and actual performance of quantum computation and sensing elements.

This instrumentation suite will enable the elucidation of chemical composition, structure, location, and size of microscopic noise sources in a superconducting quantum system, understanding the fabrication steps that introduced such noise sources, and developing fabrication approaches that minimize their presence.

I will also discuss ongoing and new research directions at the Molecular Foundry through internal staff and external user research.

8:20am **QS+2D+EM+MN+NS+VT-WeM-2 Quantum Vacuum Metrology to Advance Quantum Science Capabilities***, **Jay Hendricks**, J Ricker, K Douglass,* National Institute of Standards and Technology (NIST)*; J Fedchak, J Scherschligt,* National Institute of Sandards and Technology (NIST)

NIST is developing a series of next generation pressure and vacuum standards that will serve as a basis for key vacuum technology platforms required for emerging quantum science applications. The production of quantum sensors and devices is anticipated to require extremely demanding process control with exact knowledge of background residual gas, process chamber pressure, and accurate measurement of gas pressure feedstocks.

In 2019, National Metrology Institutes around the world worked to redefine the international system of units, the SI, such that the base units are now based on fundamental constants.

Moving forward, the next generation of pressure and standards will provide a new route of SI traceability for the pascal. By taking advantage of both the properties of light interacting with a gas and that the pressure dependent refractive index of helium can be precisely predicted from fundamental, first-principles quantum-chemistry calculations, a new route of realizing the pascal has been demonstrated. This talk will briefly cover the classical methods of realizing pressure that have served the metrology community well for the past 375 years. And then will take a deeper dive into the next generation of light-based pressure standards that will enable the elimination of mercury manometers, replacing them with a smaller, lighter, faster, and higher precision standards. From a metrology stand point, the new quantum-based SI pascal will move us from the classical force/area definition, to an energy density (joules per unit volume) definition. Should the technique be further miniaturized, it will lead to a revolution in pressure metrology, enabling a photonics-based device that serves both a gas pressure sensor and a portable gas pressure standard all in one.

NOTE: this topic is appropriate for VT sessions as well but thought it would be interesting to the broader audience that is interested in emerging quantum-based technologies that are needed to advance the field of quantum science.

8:40am **QS+2D+EM+MN+NS+VT-WeM-3 Quantum Control of Spins in Silicon Carbide with Photons and Phonons***, **David Awschalom**, S Whiteley, G Wolfowicz, K Miao,* University of Chicago **INVITED**

There are numerous efforts to embrace solid-state defects and construct quantum systems to enable new information technologies based on the quantum nature of the electron. Current studies include semiconductors with incorporated point defects, whose quantum mechanical spin properties allow a fundamentally different means to process information. In particular, interfacing solid-state defect electron spins to other quantum systems is an ongoing challenge. Here we demonstrate electrically driven coherent quantum interference in the optical transition of single divacancies, enabling new control of the spin-photon interface [1]. By applying microwave frequency electric fields, we coherently drive the excited-state orbitals and induce Landau-Zener-Stückelberg interference fringes in the resonant optical absorption spectrum. Furthermore, we develop a stroboscopic X-ray diffraction imaging technique that provides direct imaging and quantitative measurement of local strain at the nanometer scale. In conjunction with the fabrication of surface acoustic wave resonators, we mechanically drive coherent Rabi oscillations between arbitrary ground-state spin levels, including magnetically forbidden spin transitions, allowing for acoustic quantum control of local spins in silicon carbide and the exploration of spin-phonon coupling in the solid state [2]. These properties establish divacancies as strong candidates for quantum communication and hybrid system applications, where simultaneous control over optical and spin degrees of freedom is paramount.

[1] K. C. Miao *et al*., arxiv: 1905.12780

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9:20am **QS+2D+EM+MN+NS+VT-WeM-5 Tunable Control over InSb(110) Surface Conductance Utilizing Charged Defects***, **Robert Walko**, S Mueller, S Gant, J Repicky, S Tjung, E Lang, E Fuller, K Werner,* The Ohio State University*; F Bergmann,* Bergmann Messgeraete Entwicklung*; E Chowdhury, J Gupta,* The Ohio State University

In this work we present a scanning tunneling microscopy (STM) study of tip-induced switching of charge states in individual indium adatoms on the InSb(110) surface. These adatoms are deposited onto the surface by controlled voltage pulses between the STM tip and the surface. We observe them in two distinct charge states: positive and neutral. Adatom-induced band bending from the positively charged state has been observed to induce a tenfold increase in surface conductance relative to the charge neutral state, the effect of which can be observed >100nm away from the indium adatom. When the STM tip is brought sufficiently close to the defect, electrons can tunnel from the tip to the defect and cause the charge state to switch from positive to neutral. During imaging, this switching leads to a "crater" feature around the defect due to the lower conductance of the charge neutral state. The spatial extent of the crater can be tuned via the applied bias voltage, the tunneling set-point current, and photoillumination of the surface. We explain this phenomenon using a model of competing rates between the filling and emptying of the defect state, similar to dangling bonds on the Si(111) surface.

This work acknowledges funding from the DOE (# DE-SC0016379)

9:40am **QS+2D+EM+MN+NS+VT-WeM-6 Quantum Calligraphy: Writing Single-Photon Emitters in a Two-Dimensional Materials Platform***, **Matthew R. Rosenberger**,* U.S. Naval Research Laboratory*; C Dass,* Air Force Research Laboratory*; H Chuang, S Sivaram, K McCreary,* U.S. Naval Research Laboratory*; J Hendrickson,* Air Force Research Laboratory*; B Jonker,* U.S. Naval Research Laboratory

We present a paradigm for encoding strain into two dimensional materials (2DM) to create and deterministically place single photon emitters (SPEs) in arbitrary locations with nanometer-scale precision. Our material platform consists of a 2DM placed on top of a deformable polymer film. Upon application of sufficient mechanical stress using an atomic force microscope tip, the 2DM/polymer composite deforms, resulting in formation of highly localized strain fields with excellent control and repeatability. We show that SPEs are created and localized at these nanoindents, and exhibit single photon emission up to 60K. This ***quantum calligraphy*** allows deterministic placement and real time design of arbitrary patterns of SPEs for facile coupling with photonic waveguides, cavities and plasmonic structures. In addition to enabling versatile placement of SPEs, these results present a general methodology for imparting strain into 2DM with nanometer-scale precision, providing an invaluable tool for further investigations and future applications of strain engineering of 2DM and 2DM devices.

Reference: Rosenberger et al., "Quantum Calligraphy: Writing Single-Photon Emitters in a Two-Dimensional Materials Platform," *ACS Nano*, 2019, https://pubs.acs.org/doi/10.1021/acsnano.8b08730

11:00am **QS+2D+EM+MN+NS+VT-WeM-10 Challenges in Topological and Quantum Materials***, **David Alan Tennant**,* Oak Ridge National Laboratory **INVITED**

Quantum materials are rapidly advancing but still present great challenges. Topological quantum

materials in particular are receiving great attention as they provide potentially robust routes to

quantum information processing that are protected against decoherence processes. Among key

challenges are the prediction and realization of magnetic materials in the form of magnetic Weyl

semimetals and quantum spin liquids as ways of realizing exotic quasiparticles such as Majorana fermions

that can be used for application. These materials present new experimental challenges in terms of identifying their

quasiparticles and demonstrating quantum coherence in their ground states states. Here I will

show how we are using the integrated application of machine learning along with experiment and synthesis

to advance the discovery and understanding of these materials.

11:40am **QS+2D+EM+MN+NS+VT-WeM-12 Rare Earth Silicon Photonics Engineering for Quantum Applications***, A Nandi, X Jiang, D Pak,* Purdue University*; D Perry, E Bielejec,* Sandia National Laboratories*; Y Xuan, **Mahdi Hosseini**,* Purdue University

Controlling intermodal coupling between multiple excitations within a photonic material may enable the design of novel quantum photonic metamaterials exhibiting anomalous effects. Understanding the complex mode dynamics towards the engineering of system Hamiltonian has been the subject of intensive research in recent years. Here, we design an atomic lattice composed of nearly 1000 rare earth ion segments deterministically engineered in silicon photonic structures to modify the emission properties of erbium in silicon. We observe anomalous photon emission at the telecommunication wavelength from atoms geometrically arranged to reduce the propagation loss. Moreover, we map asymmetric emission lineshapes led by intermodal Fano-type interference of the atomic and photonic resonance modes. Our observation paves the way for designing active metamaterials and novel topological photonics with engineered linear and nonlinear interactions for broad applications in quantum information. Moreover, I will result for direct integration of rare earth crystals with silicon photonic chip for implementation of quantum optical memories. The approach can impact the fields of quantum communication and computation through, for example, developing superradiant single photon sources, the study of non-equilibrium many-body quantum dynamics, and engineering quantum transport in a scalable solid-state platform.

## 2D Materials
## Room A216 - Session 2D+EM+MI+NS+QS+SS-ThM
## Dopants, Defects, and Interfaces in 2D Materials
**Moderator:** Evan Reed, Stanford University

8:00am **2D+EM+MI+NS+QS+SS-ThM-1 Interfacial Engineering of Chemically Reactive Two-Dimensional Materials***, Mark Hersam,* Northwestern University **INVITED**

Following the success of ambient-stable two-dimensional (2D) materials such as graphene and hexagonal boron nitride, new classes of chemically reactive layered solids are being explored since their unique properties hold promise for improved device performance [1]. For example, chemically reactive 2D semiconductors (e.g., black phosphorus (BP) and indium selenide (InSe)) have shown enhanced field-effect mobilities under controlled conditions that minimize ambient degradation [2]. In addition, 2D boron (i.e., borophene) is an anisotropic metal with a diverse range of theoretically predicted phenomena including confined plasmons, charge density waves, and superconductivity [3], although its high chemical reactivity has limited experimental studies to inert ultrahigh vacuum conditions [4-7]. Therefore, to fully study and exploit the vast majority of 2D materials, methods for mitigating or exploiting their relatively high chemical reactivity are required [8]. In particular, covalent organic functionalization of BP minimizes ambient degradation, provides charge transfer doping, and enhances field-effect mobility [9]. In contrast, noncovalent organic functionalization of borophene leads to the spontaneous formation of electronically abrupt lateral organic-borophene heterostructures [10]. By combining organic and inorganic encapsulation strategies, even highly chemically reactive 2D materials (e.g., InSe) can be studied and utilized in ambient conditions [11].


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8:40am **2D+EM+MI+NS+QS+SS-ThM-3 Effects of Mn Doping on the Surface Electronic Band Structure and Bulk Magnetic Properties of ZnS and CdS Quantum Dot Thin Films***, **Thilini K. Ekanayaka**[1], G Gurung,* University of Nebraska-Lincoln*; G Rimal,* Rutgers University*; S Horoz,* Siirt University, Turkey*; J Tang, T Chien,* University of Wyoming*; T Paudel, A Yost,* University of Nebraska-Lincoln

Semiconducting quantum dots (QDs) are desirable for solar cells due to the ability to tune the band gap by changing the QD size without changing the underlying material or synthesis technique. Doping QDs with a transition metal is one way of further tailoring the electronic band structure and magnetic properties of QDs in order to improve overall device performance. Understanding the mechanisms causing the change in the electronic band structure and magnetic properties due to transition metal doping is important to device-by-design schemes. In this study, we measure the effects of Mn dopants on the surface electronic band structure of ZnS and CdS QDs using scanning tunneling microscopy/spectroscopy and photoemission spectroscopy. In both the ZnS and CdS systems, a decrease in band gap upon introduction of Mn is observed. Additionally, a rigid band shift was observed in ZnS upon Mn doping It is argued, using X-ray photoemission spectroscopy, that the rigid band shift is due to a hole-doping mechanism caused by the formation of Zn vacancies accompanied by a $Mn^{3+}$oxidation state which leads to the reduction in total S vacancies as compared to the undoped ZnS system. No band shift was observed in CdS upon Mn doping, but a strong sp-d hybridization takes place which results in a significant band gap reduction. Furthermore, induced midgap states originating from the Mn dopant appear in the surface electronic band structure of Mn: CdS. Measurements of the magnetization of Mn doped and undoped ZnS and CdS confirms the presence of $d^0$ ferromagnetism. The magnetization is reduced and the coercive field is increased post Mn doping which suggests the anti-ferromagnetic alignment of Mn dopant atoms. Density Functional Theory calculations support the Mn anti-ferromagnetic alignment hypothesis and a ground state with Mn in the $3^+$ valence. This study provides important information on the role of dopants and vacancies in dilute magnetic semiconductor quantum dot materials for applications in photovoltaics and spintronics.

9:00am **2D+EM+MI+NS+QS+SS-ThM-4 Interaction of Molecular $O_2$ with Organolead Halide Nanorods by Single-Particle Fluorescence Microscopy***, **Juvinch Vicente**, J Chen,* Ohio University

The photoluminescence (PL) of organolead halide perovskites (OHPs) is sensitive to its surface conditions, especially surface defect states, making the PL of small OHP crystals an effective way to report their surface states. At the ensemble level, when averaging a lot of nanocrystals, the photoexcitation of OHP nanorods under inert nitrogen ($N_2$) atmosphere leads to PL decline, while subsequent exposure to oxygen ($O_2$) results to reversible PL recovery. At the single-particle level, individual OHP nanorods photoblinks, whose probability is dependent on both the excitation intensity and the $O_2$ concentration. Combining the two sets of information, we are able to quantitatively evaluate the interaction between a single surface defect and a single $O_2$ molecule using a kinetic model. This model provides fundamental insights that could help reconcile the contradicting views on the interactions of molecular $O_2$ with OHP materials and help design a suitable OHP interface for a variety of applications in photovoltaics and optoelectronics.

9:20am **2D+EM+MI+NS+QS+SS-ThM-5 Complementary Growth of 2D Transition Metal Dichalcogenide Semiconductors on Metal Oxide Interfaces***, T Wickramasinghe, **Gregory Jensen**, R Thorat,* Nanoscale and Quantum Phenomena Institute*; S Aleithan,* Nanoscale and Quantum Phenomena Institute, Saudi Arabia*; S Khadka, E Stinaff,* Nanoscale and Quantum Phenomena Institute

A chemical vapor deposition (CVD) growth model will be presented for a technique resulting in naturally formed 2D transition metal dichalcogenide (TMD) based metal-oxide-semiconductor structures. The process is based on a standard CVD reaction involving a chalcogen and transition metal oxide-based precursor. Here however, a thin metal oxide layer, formed on lithographically defined regions of a pure bulk transition metal, serves as the precursor. X-ray diffraction and cross -sectional SEM studies show insight into the type and thickness of the metal oxide created during optimal growth conditions. The chalcogen reacts with the metal oxide, forming TMD material which migrates outward along the substrate, leading to lateral growth of highly-crystalline, mono-to-few layer, films. In addition to displaying strong luminescence, monolayer Raman signatures, and relatively large crystal domains, the material grows deterministically and selectively over large regions and remains connected to the bulk metallic patterns, offering a scalable path for producing as-grown two-dimensional materials-based devices.

9:40am **2D+EM+MI+NS+QS+SS-ThM-6 Kagome-type Lattice Instability and Insulator-metal Transition in an Alkali-doped Mott Insulator on Si(111)***, **Tyler Smith**, H Weitering,* University of Tennessee Knoxville

The 1/3 ML monolayer (ML) ‘alpha phase’ of Sn on Si(111) is a remarkable platform for the study of strong correlations in a spin ½ triangular adatom lattice. In this work, we employ an adatom doping scheme by depositing potassium onto the triangular Sn lattice. The K-atoms destabilize the parent Mott insulating phase and produce a charge-ordered insulator, revealing a rare Kagome lattice at the surface. Scanning Tunneling Microscopy and Spectroscopy reveal a phase transition from an insulating kagome lattice to a metallic triangular lattice at about 200 K. DFT band structure calculations for this kagome system [J. Ortega et al., unpublished] reveal the presence of a flat-band just below the Fermi level, making this novel system a compelling platform for hole-doping studies of magnetic and/or superconducting instabilities.

11:00am **2D+EM+MI+NS+QS+SS-ThM-10 Chemical Migration and Dipole Formation at TMD/TI Interfaces***, **Brenton Noesges**, T Zhu,* The Ohio State University*; D O'Hara,* University of California, Riverside*; R Kawakami, L Brillson,* The Ohio State University

Proximity effects at the interface between two materials can induce physical properties not present in either material alone. Topological insulators (TIs) such as $Bi_2Se_3$ with non-trivial surface states are sensitive to interface proximity effects where overlayers and adsorbates can act as a dopant source, chemically interact with the TI surface, or couple across the

[1] **National Student Award Finalist**

TI surface states leading to novel quantum phases. Transition metal dichalcogenides (TMDs), a class of 2D van der Waals materials, are a promising candidate to control this interface given the shared general hexagonal symmetry and wide range of TMD properties. However, the interface between TMDs and $Bi_2Se_3$ can be more complex than the ideal van der Waals interface. Chemical species exchange like metal cation exchange and selenium migration from substrate to growing film can impact the structure and properties of either layer. Self-assembly mechanisms have also been observed where complete metal monolayers form inside the $Bi_2Se_3$ quintuple layer [1]. We used x-ray photoelectron spectroscopy (XPS) connected in vacuo via UHV suitcase to a molecular beam epitaxy (MBE) system to investigate chemical interaction at the interface between selenide TMDs and $Bi_2Se_3$. Air-free transferring is crucial to minimize contamination at the interface and prevent oxidation in the air-sensitive TMDs. We compare the effects of ultrathin pure Mn metal overlayers and monolayer $MnSe_x$ on $Bi_2Se_3$ to pristine $Bi_2Se_3$. In the case of pure Mn metal on $Bi_2Se_3$, Bi core levels exhibit a 1.7 eV shift toward lower binding energies while the Mn core levels also show signs of Mn-Se bonding. These core level changes indicate that, in the absence of excess Se during growth, Mn pulls Se from the substrate leaving behind $Bi_2$ bilayers near the surface. Depositing a monolayer of $MnSe_x$ produces very different results than the pure metal case. $Bi_2Se_3$ core levels measured below the monolayer $MnSe_x$ film exhibit a rigid 0.8 eV chemical shift toward higher binding energies indicative of surface/interface dipole formation. The presence of this dipole is likely due to growth of primarily α-MnSe instead of the 1T-$MnSe_2$ 2D phase [2]. Scanning tunneling microscopy (STM) height maps and spectroscopy data provide further evidence of majority α-MnSe formation. XPS core level analysis combined with controlled depositions, air-free transfers and surface analysis can provide a consistent explanation of chemical diffusion and dipole formation at a TMD/TI interface. This work is supported by NSF MRSEC under award number DMR-1420451.

[1] J. A. Hagmann et al., New J. Phys. 19, 085002 (2017).

[2] D.J. O'Hara et al. Nano Lett., 18(5), 3125-3131 (2018).

11:20am **2D+EM+MI+NS+QS+SS-ThM-11 Atomically Resolved Electronic Properties of Defects in the in-plane Anisotropic Lattice of $ReS_2$**, ***Adina Luican-Mayer***, University of Ottawa, Canada

Among the layered transition metal dichalcogenides, the compounds that exhibit in-plane anisotropy are of particular interest as they offer an additional tuning knob for their novel properties. In this talk, we present experimental evidence of the lattice structure and properties of semiconducting $ReS_2$ by using scanning tunneling microscopy and spectroscopy (STM/STS). We demonstrate that rhenium atoms form diamond-shaped clusters, organized in disjointed chains and characterize the semiconducting electronic band gap by STS. When imaging the surface of $ReS_2$, we encounter "bright" or "dark" regions indicating the presence of charged defects that will electrostatically interact with their environment. By spatially mapping the local density of states around these defects, we explore their origin and electrostatic nature. Experimental results are compared with ab-initio theory.

11:40am **2D+EM+MI+NS+QS+SS-ThM-12 Charge Diminishing at the Si-$SiO_2$ System and its Influence on the Interface Properties**, ***Daniel Kropman***, *V Seeman,* Tartu University, Estonia; *A Medvids, P Onufrievs,* Riga Technical University, Latvia

The fact that a positive charge formation occurs in $SiO_2$ film during the process of Si thermal oxidation is already known, with the formation being dependent upon the oxidation conditions which involve temperature, time, and ambient conditions. This is connected by oxygen vacancies in the $SiO_2$ film and unsaturated $Si^{3\bullet}$ bonds at the interface. Until now this process has not been studied in depth at an atomic level. The purpose of the present work is to investigate the charge formation in the Si-$SiO_2$ system and its diminishing by means of the appropriate choice of oxidation conditions via EPR spectroscopy, IR spectroscopy, CV curves, TEM, and deflection measurements. Laser irradiation and ultrasonic treatment were used for the modification of interface properties. It has been established that, at an oxidation temperature that is within the range of $1125^0$C-$1130^0$C in SiO2 film with a thickness of 0.2-0.3µ at the interface, there appears a low positive or negative charge which is connected with negatively charged acceptors that are formed by Si vacancies, and the positive charge in the $SiO_2$ is compensated. The results that were obtained coincide with the point defects generation kinetic model in the Si-$SiO_2$ system which was proposed in [1] and was confirmed experimentally [2]. Integral circuit technology conditions that allow the interface charge to diminish were introduced by the semiconductor plant, ALFA (Riga, Latvia) [3]. We supposed that these results, which were obtained during long term collaboration between Estonia and Latvia, constituted a discovery that had been achieved by Si-$SiO_2$ system investigation no less than thirty years ago: the discovery of the quantum Hall effect on the Si-SiO2 structure [4].

**References**

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12:00pm **2D+EM+MI+NS+QS+SS-ThM-13 Size-independent "Squeezed" Shape of Metal Clusters Embedded Beneath Layered Materials**, *A Lii-Rosales,* Ames Laboratory and Iowa State University; *S Julien, K Wan,* Northeastern University; *Y Han,* Ames Laboratory and Iowa State University; *K Lai,* Iowa State University; *M Tringides, J Evans,* ***Patricia A. Thiel***, Ames Laboratory and Iowa State University

We have developed a continuum elasticity model for metals embedded beneath the surfaces of layered materials. The model predicts that the equilibrated cluster shape is invariant with size, manifest both by constant side slope and by constant aspect ratio (width:height ratio). This prediction is rationalized by dimensional analysis of the relevant energetic contributions. The model is consistent with experimental data for Cu and Fe clusters embedded in graphite, especially in the limit of large clusters. For comparison, we have performed a Winterbottom analysis of the equilibrium shape of an uncovered Cu cluster supported on top of graphite. The aspect ratio of the embedded cluster is about an order of magnitude higher than that of the supported cluster. Analysis of key energetics indicates that this is due to the strain energy (resistance to deformation) of the top graphene membrane, which effectively squeezes the metal cluster and forces it to adopt a relatively low, flattened shape. These insights may be useful for developing components such as metallic heat sinks or electrodes in electronic devices that use two-dimensional or layered materials.

## Manufacturing Science and Technology Group
## Room A226 - Session MS+EM+QS-ThM

### Science and Technology for Manufacturing: Neuromorphic and Quantum Computing (ALL INVITED SESSION)

**Moderators:** Nathaniel C. Cady, SUNY Polytechnic Institute, Albany, Alain C. Diebold, SUNY College of Nanoscale Science and Engineering

8:40am **MS+EM+QS-ThM-3 Materials and Fabrication Challenges for Neuromorphic and Quantum Computing Devices**, *S Olson, C Hobbs, H Chong, J Nalaskowski, H Stamper, J Mucci, B Martinick, M Zhu, K Beckmann, I Wells, C Johnson, V Kaushik, T Murray, S Novak, S Bennett, M Rodgers, C Borst, N Cady, M Liehr,* ***Satyavolu Papa Rao***, SUNY Polytechnic Institute **INVITED**

Devices for quantum computing, quantum communications and quantum sensing share many challenges in terms of the materials, their interfaces, and fabrication technologies. This presentation will quickly review the broad swath of quantum technologies that are being actively studied, while identifying synergies among them that can be exploited for efficient development of integrated quantum computing systems. Advanced process tools capable of exquisite control of the processes, materials and interfaces at 300mm wafer scale have been utilized for the fabrication of structures for quantum computing. Examples of such efforts, including structures for superconducting transmon qubits, resonators, and superconducting nanowire single photon detectors, will be discussed – with an emphasis on the materials and process control issues that needed to be tackled, while keeping manufacturability considerations always in mind. The presentation will conclude with a discussion of how advances in the fabrication of such devices for quantum computing are being applied to 'adjacent spaces' such as neuromorphic computing using superconducting optoelectronics (in partnership with AFRL-Rome and NIST Boulder).

9:20am **MS+EM+QS-ThM-5 IBM Q: Quantum Computing in the 21st Century**, ***Robert Sutor***, IBM Research **INVITED**

For almost 40 years, quantum computing has intrigued and amazed scientists and non-scientists in its future possibility for solving problems that are intractable using classical computing. Over the last three years, IBM has made real quantum computers available on the cloud so that clients, students, and researchers can begin to learn and experiment with this new way of computing. We'll see what use cases are being considered in industry, the state of quantum computing today, and how you can get on the right path to make the earliest use of this rapidly evolving technology.

11:00am **MS+EM+QS-ThM-10 Quantum Information Science at AFRL***, Michael Hayduk,* Air Force Research Laboratory **INVITED**

Recent advances in Quantum Information Science (QIS) indicate that future applications of quantum mechanics will lead to disruptive advances in capabilities for the US Air Force. Controlling and exploiting quantum mechanical phenomena will enable inertial sensors and atomic clocks that provide GPS-like positioning and timing accuracy for extended periods of time in degraded environments, communications networks with information security based on physics principles, unprecedented sensor resolution, and computers that may be able to provide exponential speedup in processing speed. To ensure that the future Air Force warfighter maintains a technological advantage, the AF must implement a QIS strategy that leads to robust, deployable quantum systems. This invited talk will discuss the recently developed Air Force Research Laboratory QIS strategy that covers the areas of timing, sensing, communications and networking, and computing. Capability development across these four areas will also be discussed.

11:40am **MS+EM+QS-ThM-12 Neuromorphic Computing: From Emerging Devices to Neuromorphic System-on-a-Chip***, **Vishal Saxena**,* University of Idaho **INVITED**

Several classes of emerging non-volatile memory (NVM) devices are currently being investigated for their application in analog implementation of artificial neural networks (ANN) hardware. The device can be two- or three-terminal and employ a wide range of material systems and associated physical mechanisms to achieve two or more non-volatile memory states. ANN hardware realizations include vector matrix multipliers (VMMs) and neural-inspired or Neuromorphic computing circuits. The NVM devices are employed in the form of crossbar or crosspoint arrays with or without selectors. In order to exploit the high-density and potential low-power operation of these devices, Analog circuit designers need to accommodate non-ideal behavior of these devices. This is particularly important for optimizing transistor-level circuit design for layout area, reliability, and static and dynamic power consumption. NVM nonidealities include device variability, low resistances offered by the two-terminal devices, finite resolution, relaxation of incremental states, limited dynamic range, and read/write endurance. This talk will provide an overview of Neuromorphic System-on-a-Chip (NeuSoC) that can be realized using emerging NVM arrays, expected device characteristics, associated circuit design challenges, and potential strategies for their mitigation. The talk will also include energy-efficiency estimation and benchmarking for NeuSoCs and provide pathways for future work in this area.

## Nanometer-scale Science and Technology Division
## Room A222 - Session NS+2D+QS-ThM

## Direct Atomic Fabrication by Electron and Particle Beams & Flash Session

**Moderators:** Canhui Wang, National Institute of Standards and Technology (NIST), Xiaolong Liu, Northwestern University

8:00am **NS+2D+QS-ThM-1 Multiprobe Scanning Tunneling Microscopy and Spectroscopy: Atomic-level Understanding of Quantum Transport in Functional Systems***, **Marek Kolmer**[1], W Ko, A Li,* Oak Ridge National Laboratory

Techniques based on multiprobe scanning tunneling microscopy (MP-STM) allow determination of charge and spin transport in variety of systems supported on surfaces of solid materials. In classical 2- and 4-probe methods STM tips are navigated by scanning electron microscope or high-resolution optical microscope typically in micrometer scales down to hundreds of nanometers. These MP-STM methods are currently regarded as universal tools for in-situ characterization of mesoscopic transport phenomena [1,2].

Such a mesoscopic experimental paradigm has recently been changed by downscaling of 2-probe STM experiments towards the atomic level [3,4]. In this case current source and drain probes are positioned in atomically defined locations with respect to the characterized nanosystems. Our experiments rely on fully STM-based tip positioning protocol with probe-to-probe separation distances reaching tens of nm [3,4]. Such probe-to-probe lateral positioning precision is combined with about pm vertical sensitivity in probe-to-system contacts. These two factors enable realization of two-probe scanning tunneling spectroscopy (2P-STS) experiments, where transport properties can be characterized by macroscopic probes kept in atomically defined tunneling conditions [4].

Here, we will apply 2P-STS methodology to probe quantum transport properties in functional systems: graphene nanoribbons (GNRs) epitaxially grown on the sidewalls of silicon carbide (SiC) mesa structures. These GNRs display ballistic transport channels with exceptionally long mean free paths and spin-polarized transport properties as proven by mesoscopic multiprobe transport experiments [5-7]. Interestingly, the nature of these ballistic channels remains an open question. We will show that 2P-STS experiments give new insight into quantum origin of the transport behaviors.

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[4] Kolmer M. et al., Nat.Commun., 10, 1573 (2019)

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This work was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility.

8:20am **NS+2D+QS-ThM-2 Light and Heavy Ions from New Non-classical Liquid Metal Ion Sources for Advanced Nanofabrication***, **Paul Mazarov**,* RAITH GmbH, Germany*; T Richter, L Bruchhaus, R Jede,* Raith GmbH*; Y Yu, J Sanabia,* Raith America*; L Bischoff,* Helmholtz Zentrum Dresden-Rossendorf, Germany*; J Gierak,* CNRS—Université Paris-Sud, France **INVITED**

Nanofabrication requirements for FIB technologies are specifically demanding in terms of patterning resolution, stability and the support of new processing techniques. Moreover the type of ion defines the nature of the interaction mechanism with the sample and thus has significant consequences on the resulting nanostructures [1]. Therefore, we have extended the technology towards the stable delivery of multiple ion species selectable into a nanometer scale focused ion beam by employing a liquid metal alloy ion source (LMAIS) [2]. This provides single and multiple charged species of different masses, resulting in significantly different interaction mechanisms. Nearly half of the elements of the periodic table are made available in the FIB technology as a result of continuous research in this area [3]. This range of ion species with different mass or charge can be beneficial for various nanofabrication applications. Recent developments could make these sources to an alternative technology feasible for nanopatterning challenges. In this contribution the operation principle, the preparation and testing process as well as prospective domains for modern FIB applications will be presented. As example we will introduce a GaBiLi LMAIS [4]. It enables high resolution imaging with light Li ions and sample modification with Ga or heavy polyatomic Bi clusters, all coming from one ion source. For sub-10 nm focused ion beam nanofabrication and microscopy, the GaBiLi-FIB or the AuSiGe-FIB could benefit of providing additional ion species in a mass separated FIB without changing the ion source.

References

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[3] J. Gierak, P. Mazarov, L. Bruchhaus, R. Jede, L. Bischoff, *Review of electrohydrodynamical ion sources and their applications to focused ion beam technology,* JVSTB 36, 06J101 (2018).

[4] W. Pilz, N. Klingner, L. Bischoff, P. Mazarov, and S. Bauerdick, *Lithium ion beams from liquid metal alloy ion sources,* JVSTB 37, 021802 (2019).

[1] **NSTD Early Career Award Finalist**

9:00am **NS+2D+QS-ThM-4 Visualizing the Interplay between Spatial and Magnetic Confinement in Graphene Quantum Dots**, ***Joseph Stroscio,*** National Institute of Standards and Technology (NIST) **INVITED**

At the heart of the wave nature of quantum mechanics is the quantization of energy due to quantum confinement, taking place when the particle's de Broglie wavelength becomes comparable to the system's length scale. In a quantum dot (QD), electrons are confined in all lateral dimensions using geometric constraints or a combination of electric and magnetic fields. Being a tunable quantum workbench, QDs have found a ubiquity of applications. Behaving as artificial atoms they have found extensive use as qubits in quantum information technologies, and tools for emulating basic models of condensed-matter physics. QDs offer an ideal platform for studying the interplay between quantum confinement, caused by spatial constraints or by large magnetic fields via cyclotron motion, and interaction effects. Recently, the ability to apply local nanometer scale gate potentials in graphene heterostructures has enabled the creation of QDs for Dirac quasiparticles. Graphene QDs are formed inside circular p-n junctions, where one has detailed control of electron orbits by means of local gate potentials and magnetic fields. We study the interplay between spatial and magnetic confinement using scanning tunneling spectroscopy measurements of the energy spectrum of graphene QDs as a function of energy, spatial position, and magnetic field. In zero field, the Dirac quasiparticles are confined by Klein scattering at large incident angle at the p-n junction boundary. The confined carriers give rise to an intricate eigenstate spectrum, effectively creating a multi-electron artificial atom. Applying a weak magnetic field results in a sudden and giant increase in energy for certain angular momentum states of the QD, creating a discontinuity in the energy spectrum as a function of magnetic field. This behavior results from a π-Berry phase associated with the topological properties of Dirac fermions in graphene, which can be turned on and off with magnetic field. With increased applied magnetic field, the QD states are observed to condense into Landau levels, providing a direct visualization of the transition from spatial to magnetic confinement in these artificial graphene atoms. With further increase in magnetic fields, an intricate interplay between Coulomb charging of compressible Landau levels separated by incompressible rings emerges, which we map as a function of energy, spatial position, and magnetic field utilizing the exceptional capabilities of scanning tunneling spectroscopy.

9:40am **NS+2D+QS-ThM-6 Using Controlled Manipulation of Molecules to Trace Potential Energy Surfaces of Adsorbed Molecules**, *O Dagdeviren, C Zhou,* Yale University*; M Todorovic,* Aalto University, Finland*;* ***Eric Altman****, U Schwarz,* Yale University

The development of scanning probe microscopy techniques has enabled the manipulation of single molecules. More recently it has been demonstrated that the forces and energy barriers encountered along the manipulation path can be quantified using non-contact atomic force microscopy (AFM). To explore the practicality of using this novel approach to experimentally measure the energy barriers an adsorbed molecule encounters as it moves across a surface decorated by other molecules including potential reaction partners, we have been studying benzene molecules on Cu (100) as a model system. We first choose a specific manipulation path and then move the tip repeatedly along this path as the tip-sample distance is reduced while recording the AFM cantilever oscillation amplitude and phase. To preserve the accurancy of the recovered tip-sample interaction potentials and forces, we use oscillation amplitudes significantly larger than the decay length of the tip-sample interaction potential are used. Operating the microscopy in the tuned-oscillator mode and analyzing the resulting cantilever oscillation amplitude and phase as functions of the spatial coordinates allows recovery of the potential energy of the interaction between the tip and the sample, the force on the tip normal to the surface, and the lateral force acting on the tip along the manipulation path, all as functions of tip vertical and lateral position with 0.01 Å resolution. In over 50 distinct maniupluation events, the molecules were either pushed, pulled, jumped to the tip, or did not move depending on the chemical environment surrounding the molecule and the chemical identity of the tip. For further insight, we have compared the experimentally measured energy landscapes and manipulation outcomes with computational results obtained using a Bayesian Optimization Structure Search protocol.

11:00am **NS+2D+QS-ThM-10 Direct Writing of Functional Heterostructures in Atomically Precise Single Graphene Nanoribbons**, ***Chuanxu Ma,*** Oak Ridge National Laboratory*; Z Xiao,* North Carolina State University*; J Huang, L Liang,* Oak Ridge National Laboratory*; W Lu,* North Carolina State University*; K Hong, B Sumpter,* Oak Ridge National Laboratory*; J Bernholc,* North Carolina State University*; A Li,* Oak Ridge National Laboratory

Precision control of interfacial structures and electronic properties is the key to the realization of functional heterostructures. Here, utilizing the scanning tunneling microscope (STM) both as a manipulation and characterization tool, we demonstrate the fabrication of a heterostructure in a single atomically precise graphene nanoribbon (GNR) and report its electronic properties[1]. The heterostructure is made of a seven-carbon-wide armchair GNR (7-aGNR) and a lower band gap intermediate ribbon synthesized bottom-up from a molecular precursor on an Au substrate. The short GNR segments are directly written in the ribbon with an STM tip to form atomic precision intraribbon heterostructures. Based on STM studies combined with density functional theory calculations, we show that the heterostructure has a type-I band alignment, with manifestations of quantum confinement and orbital hybridization. We further investigate the negative differential resistance (NDR) devices using the GNR heterostructure based double-barrier models[2]. Our computational results indicate that nanoscale engineering for NDR needs to consider atomic size effect in design and atomic precision in fabrication. This combined theoretical-experimental approach opens a new avenue for the design and fabrication of nanoscale devices with atomic precision.

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11:20am **NS+2D+QS-ThM-11 Effects of Helium and Neon Processing on 2D Material Properties**, ***Alex Belianinov,*** Oak Ridge National Laboratory*; S Kim,* Pusan National University, South Korea*; V Iberi, S Jesse, O Ovchinnikova,* Oak Ridge National Laboratory

Recent advances in CVD-growth consistently yield high quality 2D materials for large(er) scale fabrication. Monolayers of molybdenum and tungsten diselenide and suflide, graphene, and other exotic 2D materials are becoming routine in fabrication of functional electronic and optoelectronic devices. In order to attain novel functionalities, it is critical to tune and engineer defects in 2D materials directly with nanometer precision. Advances in ion beam-based imaging and nanofabrication techniques have offered a pathway to precisely manipulate 2D materials and offer a roadmap to create junctions, amorphized areas, and introduce dopants for new types of electronic devices. Here, we demonstrate the use of a focused helium and neon ion beams in a scanning helium ion microscope (HIM) in tailoring material functionality in MoSe2, WSe2, CuInP2S6 and graphene.

The helium ion microscope can "direct-write" capabilities, capable of both imaging and nanofabrication with Helium and Neon gases, thus making it an excellent candidate for processing a wide range of 2D, and conventional materials. We explore milling by the helium and neon ion beams of suspended and supported samples in order to control material's electronic and mechanical properties. We validate the results with other chemical imaging techniques such as Scanning Transmission Electron Microscopy, correlated band excitation (BE) scanning probe microscopy, and photoluminescence (PL) spectroscopy.

**Acknowledgement**

This work was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a U.S. Department of Energy (DOE) Office of Science User Facility.

11:40am **NS+2D+QS-ThM-12 Operating Molecular Propeller in Quantum Regime with Directional Control**, *Y Zhang,* ***Tolulope Ajayi,*** Ohio University*; J Calupitan,* Université de Toulouse, France*; R Tumbleson,* Ohio University*; G Erbland, C kammerer,* CEMES-CNRS, France*; S Wang,* Ohio University*; L Curtiss, A Ngo,* Argonne National Laboratory*; G Rapenne,* NAIST, Japan*; S Hla,* Ohio University

Synthetic molecular machines are fascinating and have a great promise to revolutionize a large scientific adn technology fields. The immense interest to this research area is evident by the 2016 Nobel Prize in Chemistry awarded for the design and synthesis of molecular machines. Unlike biological molecular machines, which typically have the sizes of a few microns, artificial machines operating at the nanometer scale are in the quantum regime. Here, we have developed a robust multi-component molecular propeller that enables unidirectional rotations o a materials surface when they are energized. Our propeller system is composed of a stator having a ratchet-shaped molecular gear designed to anchor on a gold surface and a rotator with three molecular blades. By means of scanning tunneling microscope imaging and manipulation, the rotation steps of individual molecular propellers are directly visualized, which confirms the unidirectional rotations of both left and right handed molecular propellers into clockwise and counterclockwise directions, respectively. Moreover, the mechanical manipulation of the molecular with the scanning probe tip further reveal detailed rotation mechanism, thereby opening a new research direction to investigate mechanical properties of the molecular machines with an atomic level precision.

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