

## **MEMS and NEMS Group Room A210 - Session MN-MoM**

### **MEMS, BioMEMS, and MEMS for Energy: Processes, Materials, and Devices I**

**Moderators:** B. Robert Ilic, National Institute for Science and Technology (NIST), Zenghui Wang, Case Western Reserve University

**8:20am MN-MoM-1 Piezoelectrics Meets Photonics – Acousto-Optic Microsystems, Gianluca Piazza, Carnegie Mellon University INVITED**  
**Advancements in thin film piezoelectric technology and the ability to define and pattern acousto-electric devices that support micron and sub-micron acoustic wavelengths have opened up new opportunities to integrate acoustic functionalities into photonic circuits. The field of optomechanics has grown from fundamental physics investigation into device applications. Acousto-optic interactions are equally interesting and will have immediate applications in facilitating miniaturization and power efficiency for radio/microwave communication, inertial sensing, photonic signal processing, optical phased arrays, and new displays for virtual/augmented/mixed reality.**

In this talk, I will present preliminary work towards the demonstration of integrated acousto-optic microsystems that take advantage of the unique properties of micro-patterned piezoelectric thin films such as sputtered aluminum nitride and single crystalline lithium niobate. The talk will focus on a couple of microsystem examples and will detail the design, fabrication and experimental demonstration of high frequency acousto-optic devices that are used for the synthesis of integrated RF oscillators or high precision and high stability gyroscope sensors.

**9:00am MN-MoM-3 On-chip Silicon Photonics Radiation Sensors, Nikolai Klimov, Z Ahmed, R Fitzgerald, L Cumberland, I Pazos, R Tosh, National Institute of Standards and Technology (NIST)**

The last few decades have witnessed an exponential growth in photonics, driven in part by improvements in micro-electronics fabrication techniques and by increasing adoption of photonics components by the telecommunications industry. As a result, a wide variety of photonics-based devices have been recently proposed and developed [1-4]. These photonic sensors are particularly valuable due to their micro-/nanoscale footprint, ultra-high sensitivity, low power consumption, and tolerance to harsh environmental variables. One potential application of photonic sensors is ionizing radiation dosimetry. At present, primary standards for absorbed dose are based on large ( $m^3$ ) water calorimeters used to link the absorbed energy from a large uniform radiation beam to the temperature rise in a  $\sim 0.5$ -mm sized thermistor probe. The realization of this standard requires radiation-beam uniformity on the order of centimeters. On the other hand, rapidly evolving medical and industrial applications are demanding a deployable solution capable of detecting ionizing radiation on a millimeter to micrometer scale. To address industry demand, National Institute of Standards and Technology (NIST) has recently started a program to develop the next generation radiation dose primary standards. The new proposed standard, built on a nano-photonic chip, will leverage nano-photonics and frequency metrology to provide a field-deployable solution. Our radiation sensors are based on high-Q silicon photonic resonators such as ring resonators and photonic crystal cavities. We have recently demonstrated [5] that these sensors can withstand 1 MGy (1 Gy = 100 Rad) absorbed dose in ca. 1 MeV gamma- and electron-beam irradiations with negligible degradation to device performance. In this presentation we will give an overview of the NIST photonic dosimetry program and its most recent developments. We will explain design, nanofabrication, packaging and interrogation of our devices. We will also show our preliminary results on real-time photonic calorimetry measurements in on/off cycles of the electron beam provided by a Van de Graaff accelerator at nominal dose rate of kGy/s. Comparison of the device response with the output of finite-element modelling of heat transport and dose measurements obtained by co-irradiated alanine pellets (analyzed via EPR) will also be discussed.

[1] B. Guha et al., *Opt. Lett.* 37 (212) 2253–2255.

[2] Oates, L.W. Burgess, *Anal. Chem.* 84 (2012) 7713–7720.

[3] H. Xu, et al., *Opt. Express.* 22 (214) 3098–3104.

[4] N.N. Klimov, et al., *Sensors and Actuators A*, 269 (2018) 308–312.

[5] Z. Ahmed, et al., *Sci. Rep.* 8 (2018) 13007.

**9:20am MN-MoM-4 Synthesis and Characterization of Nanoscale 3 dimensional Plasmonic Architectures, Grace Pakeltis, E Mutunga, University of Tennessee Knoxville; Z Hu, D Masiello, University of Washington; J Idroba, Oak Ridge National Laboratory; H Plank, Graz University of Technology, Austria; J Fowlkes, Oak Ridge National Laboratory; P Rack, University of Tennessee Knoxville**

New breakthroughs and better understanding in the underlying theory of plasmonics has led to an increased demand for advanced design, synthesis and device integration strategies for plasmonic nanomaterials. Three-dimensional plasmonic nanostructures have the ability to advance applications such as ultra-fast communication, high density memories, and sensing while enabling further investigation into plasmonic physical phenomena. In this study, we illustrate a nanoscale synthesis process which utilizes a hybrid of direct-write 3D nanoprinting and thin film deposition to fabricate complex, free-standing plasmonic nanostructures for the investigation of 3D plasmonics. Focused electron beam induced deposition is used to deposit non-plasmonic 3D scaffolds, which are subsequently isolated with a conformal  $\text{SiO}_2$  layer and coated with a plasmonic materials, specifically Au, to create functional 3D plasmonic nanostructures. A variety of single and dimer structures were fabricated and low-loss electron energy loss spectroscopy was utilized to characterize their full plasmonic spectra with nanoscale resolution. Complementary electron discrete dipole approximation simulations were performed to elucidate the resultant consequent electric and magnetic field distributions. This work demonstrates the flexibility FEBID scaffolds offer for the advancement of new 3D devices for applications and fundamental studies of plasmonic nanomaterials.

**9:40am MN-MoM-5 2D Raman Imaging and Characterization of Surface Acoustic Waves on GaAs Substrates, Brian Douglas Rummel, G Heileman, University of New Mexico; M Henry, Sandia National Laboratories; S Han, University of New Mexico**

We have fabricated Surface Acoustic Wave (SAW) devices on a GaAs (110) substrate to demonstrate the capability of 2D Raman microscopy to image and characterize acoustic waves traveling on the surface of a piezoelectric substrate. SAW devices are typically utilized in sensors and rf filters, and developing a facile technique to image the transmitted signal would be useful in characterizing device operation and optimization. SAWs are generated using a two-port interdigital transducer (IDT) platform, modified to produce free surface standing waves. These standing waves provide a means to differentiate nodes and antinodes of the acoustic wave. The frequency of SAWs does not easily allow *in situ*, real-time imaging of the waves. However, we make use of Raman peak broadening that corresponds to an averaging of the peak shifts over the integration time of the spectrometer. We have derived an analytical model to fit the peak broadening and effectively calculate the maximum strain induced by the acoustic waves, thus allowing one to characterize the SAWs and measure surface displacements on the order of picometers. The application of this research for the strain-induced fabrication of highly ordered nano/micro structures in III-V semiconductors will also be discussed.

**10:00am MN-MoM-6 Impacts of Stress and Dissipation in van der Waals Interfaces on 2D Material Nanoelectromechanical Systems, SunPhil Kim, A van der Zande, University of Illinois at Urbana-Champaign**

Two-dimensional materials such as graphene and  $\text{MoS}_2$  represent the ultimate limit of both nanoelectronic and nanoelectromechanical systems due to their intrinsic molecular scale thickness. While 2D materials exhibit many useful properties, many of the most exciting phenomena and applications arise at the van der Waals interface. Electrically, the van der Waals interface enables the constructing of heterostructures and molecular scale electronics. Mechanically, the van der Waals interface displays superlubricity[1] or solitons[2] depending on whether the interface is aligned. A fascinating question is how the van der Waals interface affects the mechanical properties of 2D membranes. Answering this question is important to incorporating 2D heterostructure electronics into diverse applications such as highly tunable nanoelectromechanical systems from suspended 2D membranes, stretchable electronics from crumpled 2D materials, and origami/kirigami nano-machines.

In this study, we explore the impact of the van der Waals interface by comparing mechanical resonance of electrostatically contacted circular drumhead resonators made from atomic membranes of monolayer graphene to commensurate (Bernal stacked) bilayers, incommensurate (twisted) bilayer, and graphene- $\text{MoS}_2$  heterostructures (2D bimorph).

For Bernal stacked bilayer, we observe the creation and destruction of individual solitons manifesting as stochastic jumps in the mechanical

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resonance frequency tuning. We find individual dislocation creation and destruction of single solitons lead to shifts in membrane stress of  $< 7$  mN/m or an in-plane interlayer slip distance of  $< 0.7$  Å. We observe similar jumps in the few layer graphene and heterostructure, but not in the twisted bilayer.

For twisted bilayer, temperature and amplitude dependent studies reveal that the resonators show a factor of 3 higher dissipation rate, leading to different nonlinear behaviors compared to monolayer graphene and Bernal stacked bilayer resonators.

These results show that van der Waals interfaces strongly affect stress and dissipation of many multilayer 2D atomic membranes; an important consideration in engineering 2D nanomechanical devices.

[1]Dienwiebel, M.; Verhoeven, G. S.; Pradeep, N.; Frenken, J. W. M.; Heimberg, J. A.; Zandbergen, H. W., Superlubricity of graphite. *Phys Rev Lett* **2004**,92(12).

[2]Alden, J. S.; Tsen, A. W.; Huang, P. Y.; Hovden, R.; Brown, L.; Park, J.; Muller, D. A.; McEuen, P. L., Strain solitons and topological defects in bilayer graphene. *P Natl Acad Sci USA* **2013**,110(28), 11256-11260.

10:40am **MN-MoM-8 Nanomechanical Sensing for the Life Sciences, Montserrat Calleja**, IMN-CSIC, Spain **INVITED**

Physical and, among them, mechanical properties of biological entities as cells, bacteria, viruses and biomolecules are valuable cues to better understand human diseases. Still, this has remained an underexplored route for the development of novel biosensing and diagnostic strategies. Biosensors based on nanomechanical systems are best suited to respond to the demand for accurate physical characterization of biofilms, biomolecules and single cells. The continuous downscaling of such devices from micro- to nano- scale is providing a drastic improvement in their mass resolution, while the robustness of nanomechanical biosensors for high throughput immunodetection has reached the demands of clinical applications. Interestingly, other physical parameters than the added mass of the biological targets are at reach for nanomechanical systems. We have recently observed that thin films of DNA demonstrate a Young's modulus tuning range of about 10 GPa, by simply varying the environment relative humidity from 0% up to 70%; while upon hybridization with the complementary strand, the DNA self-assembled monolayers significantly soften by one order of magnitude. Thus, we have demonstrated direct detection without prior purification or amplification of DNA sequences for gene-based identification of pathogens and antibiotic resistances. Also, the mass, position and stiffness of analytes arriving the resonator can be extracted from the adsorption-induced eigenfrequency jumps. We have proposed that this approach serves for identification of large biological complexes near their native conformation, a goal that is beyond the capabilities of conventional mass spectrometers. The capability to describe the analytes that arrive to the resonator by two orthogonal coordinates, the mass and the stiffness, clearly enhances the selectivity of nanomechanical spectrometry and it opens the door to relevant biomedical applications, as now the important role of mechanical properties in biological processes and in pathogenic disorders is becoming increasingly clear. In this talk, several avenues to advance nanoresonators for multiparameter fingerprinting of single proteins, cells, viruses and bacteria will be reviewed.

11:20am **MN-MoM-10 Neutral Mass Spectrometry of Metallic Nanoparticles with Optomechanical Resonators, Marc Sansa, M Defoort, M Hermouet, L Banniard, A Fafin, M Gely**, Université Grenoble Alpes, CEA, LETI, France; *I Favero*, Centre de Nanosciences et de Nanotechnologies, CNRS, Université Paris-Sud, Université Paris-Saclay, France; *G Jourdan*, Université Grenoble Alpes, CEA, LETI, France; *A Brenac*, Université Grenoble Alpes, CEA, CNRS, Grenoble INP, INAC-Spintec, France; *S Hentz*, Université Grenoble Alpes, CEA, LETI, France

Nanomechanical resonators have shown record performance in mass or force sensing thanks to their miniature sizes. Pioneering works have shown single protein mass spectrometry (MS) could be performed with nanoresonators (1). It was recently demonstrated that they are particularly well suited for the analysis of high-mass species like virus capsids (~100MDa), out of reach for any commercial instrument as of today (2). In parallel, cavity-based nano-optomechanical resonators have shown exceptional displacement sensitivities (3), opening new avenues to improve the limit of detection of nanomechanical sensors (4). Here we report the first proof of concept of mass spectrometry with a nano-optomechanical resonator, made possible by a novel resonator geometry, the combination of optomechanics with electrical actuation and advances in fabrication and assembly of the sensor.

Taking advantage of the optomechanical detection, we use an ultra-thin planar sensor geometry. It displays several advantages compared to commonly used 1D-like resonators: the capture area is increased threefold while maintaining a similar mass resolution. Additionally, this planar membrane resonator is designed to be insensitive to particle position, shape or stiffness, avoiding the need for multi-mode operation (5). The resonators are fabricated using the first Very Large Scale Integration process for optomechanics, which allows the combination of standard photonic components (grating couplers, waveguides, optical cavities), electrical actuation of the resonator and a protection layer covering the optical and electrical features.

Our process and design also allow optical packaging in order for our sensor to be portable and usable in any vacuum system with optical and electrical input/outputs, such as a sputtering system containing a standard Time-of-Flight (TOF) mass spectrometer (6). This set-up allows the generation of particles of controllable mass, and the comparison of optomechanical and TOF mass spectrometry in situ. We show that the measured mass is equivalent with both techniques, while optomechanical detection is more performant at higher masses (>5 MDa), where TOF becomes less efficient. This work represents the first step towards the optomechanical addressing of large sensor arrays, which combine the advantages of nanomechanical sensors with reduced analysis times comparable to those of conventional MS.

1. M.S. Hanay et al. *Nat. Nanotechnol.* (2012)
2. S. Dominguez-Medina et al. *Science* (2018)
3. A. Schliesser et al. *New J. Phys.* (2008)
4. A. Venkatasubramanian et al. *Nano Lett.* (2016)
5. E. Gil-Santos et al. *Nat. Nanotechnol.* (2010)
6. E. Sage et al. *Nature Communications* (2018)

11:40am **MN-MoM-11 Mass Calibration of Nanomechanical Resonators from Electrical Measurements for Mass Spectrometry Applications, Bogdan Vysotskyi**, CEA/LETI-University Grenoble Alpes, France; *S Lai*, CEA/IRIG-University Grenoble Alpes, France; *M Defoort, M Sansa*, CEA/LETI-University Grenoble Alpes, France; *K Clement*, CEA/IRIG-University Grenoble Alpes, France; *M Gely*, CEA/LETI-University Grenoble Alpes, France; *C Masselon*, CEA/IRIG-University Grenoble Alpes, France; *S Hentz*, CEA/LETI-University Grenoble Alpes, France

Nanomechanical resonators have recently shown their potential to extend mass spectrometry towards a mass range inaccessible to commercial spectrometers [1]. The frequency shift-to-particle mass conversion requires precise knowledge of the resonator's effective mass. When using a single resonator, uncertainty on the effective mass translates into a shift into central mass of the measured mass profile. If this resonator can be used for a large amount of time, time and effort can be spent into proper morphological characterization such as scanning electronic microscopy or local stress measurement. While these techniques can be suitable for MEMS-type devices [2], they prove much more complex and less effective in the case of nanomechanical resonators due to limited precision (*c.a.* 5 to 10nm). Moreover, the issue becomes way more acute when using arrays of resonators [3]: in this case, effective mass uncertainty and variability within the array leads to shifts in central mass, but also changes in mass profile. Lastly, routine particle measurements demand frequent changes in devices and time-effective calibration techniques are required. This crucial issue for mass spectrometry applications is very little discussed in the literature, or is addressed with complex procedures [4]. FEM simulations show that two main parameters impact effective mass assessment in the case of our monocrystalline silicon resonators (160nm thickness, 300nm width and *c.a.* 10µm long): width and residual plane stress. The resonance frequencies of all resonators in the array are measured, thus both deviation from the theoretical frequency spacing and absolute frequency of our 20 resonators in the array are used for calibration of effective mass. A two-step optimization routine is used in conjunction with a physical model and internal stress and beam width are deduced. With this method an extremely low absolute mass error (<1%) is demonstrated to be reached. This non-destructive technique based on electrical measurement is amenable to the future use of very large arrays (>1000 resonators) for very short analysis time. This method can be extended for non-destructive characterization of nanomechanical resonators for different applications.

- [1] S. Dominguez-Medina et al., *Science* 362, 918-922 (2018)
- [2] A. Brenes et al., *Mechanical Systems and Signal Processing* 112, 10-21 (2018)

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[3] E. Sage et al., Nature Communications 9 : 3283 (2018)

[4] O. Malvar et al., Nature Communications 7 : 13452 (2016).

## 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 utmost 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  $\mu$ s. 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  $\mu$ s – 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](http://www.wacqt.se)

[2] [www.opensuperq.eu](http://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 ( $\text{Nb}_x\text{Ti}_{1-x}\text{N}$ ) 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

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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.

## Thin Films Division

### Room A122-123 - Session TF+EM+MI+MN+OX+PS-MoM

#### Functional Thin Films: Ferroelectric, Multiferroics, and Magnetic Materials

**Moderators:** Christophe Vallee, LTM - MINATEC - CEA/LETI, France, Jessica Kachian, Intel Corporation

8:20am **TF+EM+MI+MN+OX+PS-MoM-1 A Room-Temperature Magnetolectric Multiferroic made by Thin Film Alchemy**, *D Schlom, Megan Holtz*, Cornell University **INVITED**

Materials that couple strong ferroelectric and ferromagnetic order hold tremendous promise for next-generation memory devices. Meticulous engineering has produced novel ferroelectric and multiferroic materials, although known single-phase multiferroics remain limited by antiferromagnetic or weak ferromagnetic alignments, by a lack of coupling between the order parameters, or by having properties that emerge only well below room temperature. Here we construct single-phase multiferroic materials in which ferroelectricity and strong magnetic ordering are coupled near room temperature. Starting with hexagonal  $\text{LuFeO}_3$ —a geometric ferroelectric with planar rumpling—we introduce individual monolayers of ferrimagnetic  $\text{LuFe}_2\text{O}_4$  within the  $\text{LuFeO}_3$  matrix, that is,  $(\text{LuFeO}_3)_m/(\text{LuFe}_2\text{O}_4)_1$  superlattices. The rumpling of the  $\text{LuFeO}_3$  drives the ferrimagnetic  $\text{LuFe}_2\text{O}_4$  into a ferroelectric state, reducing the  $\text{LuFe}_2\text{O}_4$  spin frustration. This increases the magnetic transition temperature to 281K for  $m=9$ . Moreover, the ferroelectric order couples to the ferrimagnetism, enabling direct electric-field control of magnetism at 200 kelvin. Further, charged ferroelectric domain walls align at  $\text{LuFe}_2\text{O}_4$  layers, resulting in charge transfer which increases the magnetic moment. We are currently pursuing higher temperature multiferroics by incorporating cubic spinels with high magnetic ordering temperatures, such as  $\text{CoFe}_2\text{O}_4$ , into the  $\text{LuFeO}_3$  matrix. Our results demonstrate a design methodology for creating higher-temperature magnetolectric multiferroics through epitaxial engineering.

9:00am **TF+EM+MI+MN+OX+PS-MoM-3 Magnetic Losses in FeGa/NiFe/Al<sub>2</sub>O<sub>3</sub> Laminates for Strain-Mediated Multiferroic Micro-Antenna Applications**, *Kevin Fitzell, A Acosta, C Rementer, D Schneider, Z Yao*, University of California, Los Angeles; *C Dong*, Northeastern University; *M Jamer, D Gopman, J Borchers, B Kirby*, National Institute of Standards and Technology (NIST); *N Sun*, Northeastern University; *Y Wang, G Carman, J Chang*, University of California, Los Angeles

The ability to reduce the size of antennae would enable a revolution in wearable and implantable electronic devices. Multiferroic antennae, composed of individual ferromagnetic and piezoelectric phases, could reduce antenna size by up to five orders of magnitude through the efficient

coupling of magnetization and electric polarization via strain. This strategy requires a material with strong magnetoelastic coupling and acceptable magnetic losses at high frequency.

Galfenol ( $\text{Fe}_{84}\text{Ga}_{16}$  or FeGa) is a promising candidate material due to its large magnetostriction (200  $\mu\epsilon$ ), large piezomagnetic coefficient (5 ppm/Oe), and high stiffness (60 GPa), but it is highly lossy in the GHz regime. On the other hand, Permalloy ( $\text{Ni}_{81}\text{Fe}_{19}$  or NiFe) is a soft magnetic material that has very low loss in the GHz regime, with a ferromagnetic resonance (FMR) linewidth of 10 Oe, but almost no magnetostriction. In this work, nanoscale laminates containing alternating layers of FeGa and NiFe were fabricated via DC magnetron sputtering to combine the complementary properties of the two magnetic phases, resulting in a composite material with a small coercive field, narrow FMR linewidth, and high permeability (Rementer et al., 2017). Optical magnetostriction measurements confirmed that these laminates retain the large saturation magnetostriction of FeGa (200  $\mu\epsilon$ ) while enhancing the piezomagnetic coefficient (7 ppm/Oe), allowing for optimal piezomagnetic actuation at substantially reduced magnetic bias fields. Furthermore, multiferroic composites incorporating these magnetic laminates were studied via polarized neutron reflectometry, demonstrating uniform rotation of the individual layers' magnetization with an applied electric field across distances much larger than the exchange length of either material.

Due to the metallic nature of these FeGa/NiFe multilayer composites, however, resulting devices would be inefficient due to the generation of eddy currents at high frequency. To mitigate these losses, ultrathin layers of  $\text{Al}_2\text{O}_3$  were incorporated into the multilayer materials to reduce the conductivity and mitigate the generation of eddy currents. The effect of  $\text{Al}_2\text{O}_3$  thickness, FeGa:NiFe volume ratio, and multilayer architecture on the soft magnetic properties was also studied, resulting in a 50% reduction in the FMR linewidth. Optimized magnetic laminates were shown to exhibit a small coercive field (<20 Oe), narrow ferromagnetic resonance linewidth (<50 Oe), and high relative permeability (>500) while maintaining excellent magnetoelastic coupling, showing great promise for the use of FeGa/NiFe/ $\text{Al}_2\text{O}_3$  laminates in strain-mediated micro-scale communications systems.

9:20am **TF+EM+MI+MN+OX+PS-MoM-4 Multiferroic Gd-substituted HfO<sub>2</sub> Thin Films**, *John Hayden, F Scurti, J Schwartz, J Maria*, Pennsylvania State University

Modern ferroelectric technologies utilize perovskite structured materials, which have limited Si compatibility and modest bandgaps requiring thick films to reduce leakage current, hindering their implementation in realizable thin film devices.  $\text{HfO}_2$  has been extensively researched as a gate dielectric thin film with excellent Si processing compatibility and has recently been found to exhibit ferroelectricity induced by a combination of impurity substitution, mechanical confinement by capping, intergranular surface area, and film thickness effects. This work investigates the microstructural characteristics, the ferroelectric response, and the potential for concomitant magnetic properties in sputtered Gd:HfO<sub>2</sub> thin films.

Gd-substituted HfO<sub>2</sub> thin films are a promising candidate as a multiferroic material, due to the presence of the magnetically active Gd<sup>3+</sup> ion. Though substituting with Gd is known to induce ferroelectricity in HfO<sub>2</sub>, the magnetic properties of Gd:HfO<sub>2</sub> have yet to be studied in depth. In this study, Gd:HfO<sub>2</sub> films are fabricated on TaN substrates by radio frequency sputtering of a composite Gd metal and HfO<sub>2</sub> oxide target in a mixed Ar and O<sub>2</sub> atmosphere. Grazing incidence x-ray diffraction is used to evaluate the suppression of the paraelectric monoclinic phase and stabilization of the ferroelectric orthorhombic phase. Electrical polarization measurements are used to study the room temperature spontaneous polarization in TaN/Gd:HfO<sub>2</sub>/TaN metal-insulator-metal capacitors. Surface morphology of the films is characterized using atomic force microscopy, while magnetic properties are measured by variable temperature magnetometry. Initial magnetometry shows that Gd-substituted HfO<sub>2</sub> exhibits remnant magnetization at room temperature.

The scalability and simplicity of Gd:HfO<sub>2</sub>, if it exhibits magnetolectric coupling, make it an attractive model system for future developments in thin film multiferroics, having potential impacts for spintronics and other magneto-electronic devices.

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9:40am **TF+EM+MI+MN+OX+PS-MoM-5 Epitaxial Growth of Antiferromagnetic NiO Films by Off-axis Sputtering for Spintronic Devices**, *A Churikova, G Beach*, Massachusetts Institute of Technology; *Larry Scipioni, A Shepard, J Greer, T Newhouse-Ilige*, PVD Products, Inc.

High-quality epitaxial growth of antiferromagnetic thin films is essential for future spintronic devices, as it allows small antiferromagnetic domain sizes and efficient electrical manipulation of domain walls via reading and writing currents. Antiferromagnetic materials are candidates for ultrafast operation due to THz antiferromagnetic spin dynamics, high packing densities due to the absence of stray magnetic fields, and stability due to insensitivity to external magnetic fields [1,2]. Meanwhile, the long spin diffusion lengths [3] and theoretically predicted superfluid transport of spin currents [4] in antiferromagnetic insulators are crucial for low-power device operation. The electrical control of magnetic spin textures has been thus far realized in epitaxially grown NiO on MgO substrates [5] and ferrimagnetic maghemite ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>) and magnetite (Fe<sub>3</sub>O<sub>4</sub>) thin films [6].

We report the preparation of antiferromagnetic NiO thin films with (111) orientation on *c*-plane sapphire (1000) substrates by off-axis RF magnetron sputtering from a NiO target. The off-axis angle was 45°, and the sputtering pressure was 5 mTorr. Samples were grown with thicknesses ranging from 5 – 50 nm, and with growth temperatures from room temperature to 600°C, to determine optimum conditions. Structural characterization by x-ray diffraction demonstrates a high degree of epitaxy across a range of deposition temperatures and thicknesses. The deposition temperature and thickness dependence of epitaxial quality is investigated, with a characterization of the strain state, mosaicity, and crystallographic relationship between substrate and film. Evidence for antiferromagnetic order forming domains in NiO is provided via magnetic characterization of the films. Our results are essential for the optimization of the fabrication of high quality epitaxial antiferromagnetic films for practical spintronics devices.

[1] J. Železný, P. Wadley, K. Olejník, A. Hoffmann, and H. Ohno, *Nat. Phys.* 14, 220 (2018)

[2] V. Baltz, A. Manchon, M. Tsoi, T. Moriyama, T. Ono, and Y. Tserkovnyak, *Rev. Mod. Phys.* 90, 015005 (2018).

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[6] L. Baldrati, A. Ross, T. Niizeki, C. Schneider, R. Ramos, J. Cramer, O. Gomonay, M. Filianina, T. Savchenko, D. Heinze, A. Kleibert, E. Saitoh, J. Sinova, and M. Kläui, *Phys. Rev. B* 98, 024422 (2018).

10:00am **TF+EM+MI+MN+OX+PS-MoM-6 Structural and Magnetic Properties of CoPd Alloys for Non-Volatile Memory Applications**, *S Gupta, J Abugri, B Clark*, University of Alabama; *P Komninou*, Aristotle University of Thessaloniki; *Sujan Budhathoki, A Hauser, P Visscher*, University of Alabama

A study of perpendicular magnetic anisotropy (PMA) CoPd alloys is presented as a simple means of pinning MgO-based perpendicular magnetic tunnel junctions (pMTJs) for spin transfer torque magnetic tunnel junction (STT-MRAM) applications. A compositional study of the Co<sub>x</sub>Pd<sub>100-x</sub> alloys at 50 nm thickness showed that the maximum coercivity and anisotropy was found for Co<sub>25</sub>Pd<sub>75</sub>. Perpendicular magnetic tunnel junction stacks were deposited using different compositions of CoPd. Current-in-plane tunneling measurements indicated that the TMR values roughly correlated with the coercivity and anisotropy of the single layers. A thickness study indicated that the alloy was fully perpendicular for thicknesses as low as 20 nm. Various seed layers were employed to optimize the coercivity of the Co<sub>25</sub>Pd<sub>75</sub> layer. Magnetometry, X-ray diffraction (XRD), scanning electron microscopy (SEM) and high resolution transmission electron microscopy studies were carried out to relate the magnetic and structural properties of these layers. These studies showed that the highest coercivity Co<sub>25</sub>Pd<sub>75</sub> was achieved on a seed layer of Ta/Pd which helped to crystallize the CoPd layer in an fcc (111) orientation.

10:40am **TF+EM+MI+MN+OX+PS-MoM-8 Size Effects of the Electromechanical Response in Ferroic Thin Films: Phase Transitions to the Rescue**, *Nazanin Bassiri-Gharb*, Georgia Institute of Technology  
**INVITED**

Silicon-integrated ferroelectric thin films have been leveraged over the last two decades for fabrication of high performance piezoelectric microelectromechanical systems (MEMS) devices. Ceramic Pb(Zr<sub>x</sub>Ti<sub>1-x</sub>)

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x)O<sub>3</sub>(PZT) thin films have been often the material of choice, due to their large electromechanical response, especially at morphotropic phase boundary compositions (MPB at  $x \sim 0.52$ ), where co-existence of multiple crystallographic distortions can enhance extrinsic electromechanical contributions. However, ferroelectric thin films suffer from extrinsic size effects that lead to deteriorated piezoelectric properties in thin and ultrathin films. Here we report on different strategies for processing of thin films with enhanced piezoelectric response with respect to traditionally processed PZT thin films.

Specifically, we will discuss preparation of superlattice-like polycrystalline PZT thin films through chemical solution depositions, polycrystalline relaxor-ferroelectric thin films (PMN-PT), and finally alternative non-ferroelectric compositions, where the electric field-induced phase transitions can result in substantial enhancement in thinner films, even where traditional

11:20am **TF+EM+MI+MN+OX+PS-MoM-10 Ferroelectrics Meet Ionics in the Land of van der Waals**, *S Neumayer*, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory; *J Brehm*, Vanderbilt University; *M McGuire*, Oak Ridge National Laboratory; *M Susner*, Air Force Research Laboratory; *E Eliseev*, National Academy of Sciences of Ukraine; *S Jesse*, *S Kalinin*, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory; *A Morozovska*, National Academy of Sciences of Ukraine; *S Pantelides*, Vanderbilt University; *N Balke*, **Petro Maksymovych**, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Van der Waals crystals of metal thiophosphates can be thought of as derivatives of transition metal dichalcogenides where 1/3 of metal atoms is replaced with diphosphorous, thereby stabilizing the remaining 2/3 of metal ions in low oxidation states.1 Consequently, thiophosphates enable ultrathin magnetic, ferroelectric and Mott insulating materials, in q2D materials while also providing new opportunities for multifunctional interfaces .

Of particular interest is CuInP<sub>2</sub>S<sub>6</sub>, where ferroelectricity emerges out of ionically conducting state .2,3 In this work, we discuss unusual and perhaps anomalous properties observed in CuInP<sub>2</sub>S<sub>6</sub> in both states.

CuInP<sub>2</sub>S<sub>6</sub> exhibits giant negative electrostriction ( $Q_{33} = -3.2 \text{ m}^4/\text{C}^2$ ), which leads to large piezoelectric coefficients despite small polarization values and increase of Tc with applied pressure. It's the only material other than polymer PVDF for which such behavior is experimentally confirmed. Density functional theory reveals that the reason for negative electrostriction is a slight movement of Cu ions into the van der Waals gap due to anharmonicity of the potential well.4 Moreover, under high compressive strain, Cu starts to form interlayer bonds with sulfur across the van der Waals gap, leading to an additional phase of high polarization. Consequently, the potential distribution exhibits 4 instead of the usual two minima - a quadruple well, that is precisely tunable by strain. In the paraelectric state above ~70°C, Cu ion mobility drastically increases. Intriguingly, Cu can be reversibly extracted out of the lattice without visible damage. Finally, the selenide sibling CuInP<sub>2</sub>Se<sub>6</sub>, exhibits a lower transition temperature and propensity toward antiferroelectric ordering under the effect of depolarizing fields. In this material, we have for the first time observed piezoelectric response confined to domain walls (opposite to ferroelectrics), fulfilling the long-standing predictions for polar antiferroelectric domain walls and providing a new model system for emergent properties of topological defects in ferroic order parameter fields.

Research sponsored by Division of Materials Science and Engineering, Basic Energy Sciences, US Department of Energy. Microscopy was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

1Susner et al, *Adv. Mater.* 29,1602852 (2018)

2Neumayer et al, *Phys. Rev. Materials* 3, 024401 (2019)

3Balke et al, *ACS Appl. Mater. Interfaces* 10, 27188 (2018)

4Brehm et al, in review

11:40am **TF+EM+MI+MN+OX+PS-MoM-11 Adsorption-controlled Epitaxial Growth of the Hyperferroelectric Candidate LiZnSb on GaSb (111)**, *D Du, P Strohbeen*, University of Wisconsin - Madison; *H Paik*, Cornell University; *C Zhang, P Voyles, Jason Kawasaki*, University of Wisconsin - Madison

A major challenge for ferroelectric devices is the depolarizing field, which competes with and often destroys long-range polar order in the limit of

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ultrathin films. Recent theoretical predictions suggest a new class of materials, termed hyperferroelectrics [1], should be immune to the depolarizing field and enable ferroelectric devices down to the monolayer limit. Here we demonstrate the epitaxial growth of hexagonal LiZnSb, one of the hyperferroelectric candidate materials, on GaSb (111) substrates. Due to the high volatility of all three atomic species, we find that stoichiometric films can be grown in a thermodynamically adsorption-controlled window, using an excess zinc flux. Outstanding challenges remain in controlling the point defects of LiZnSb and in controlling polytypism. While the films primarily grow in a hexagonal “stuffed wurtzite” phase (space group  $P6_3mc$ ), which has the desired polar structure, there exists a competing cubic “stuffed zincblende” polymorph that is nonpolar ( $F-43m$ ). We will discuss our strategy towards controlling defects and polytypism in LiZnSb, which is based in large part on the wurtzite – zincblende polytypism observed in InAs. We will also present preliminary electrical measurements on phase pure ferroelectric capacitor structures.

This work was supported by the Army Research office (W911NF-17-1-0254) and the National Science Foundation (DMR-1752797).

[1] K. F. Garrity, K. M. Rabe, and D. Vanderbilt, Phys. Rev. Lett. **112**, 127601(2014).

## 2D Materials

### Room A226 - Session 2D+AP+EM+MI+MN+NS+PS+TF-MoA

#### Nanostructures including Heterostructures and Patterning of 2D Materials

**Moderator:** Deep Jariwala, University of Pennsylvania

##### 1:40pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-1 Tailoring and Patterning 2D Material Interfaces Through Chemical Functionalization, *Arend van der Zande*, University of Illinois at Urbana-Champaign **INVITED**

Two-dimensional materials are all surface, so any change in the surface chemistry affects the entire material. This offers a challenge and an opportunity to engineering the material properties and new device behavior. There are many strategies to altering the chemical structure of 2D materials, yet one of the most successful is the chemical functionalization with low energy plasmas such as hydrogen and fluorine. Functionalization enables phase changes within materials to dramatically alter their properties, can be applied post synthesis and device fabrication, and is compatible with lithography for spatial patterning. Most studies of chemical functionalization focus on single functionalization of single 2D materials, yet there are many opportunities when applying the principles of chemical functionalization to spatially engineer the properties through in plane interfaces or out of plane in heterostructures.

First, we will examine selective etching with XeF<sub>2</sub> to pattern heterostructures using graphene etch stops. These techniques are self-limiting, yet scalable, and enable the patterning of 2D heterostructures into 3D multilayer circuitry. Moreover, devices like encapsulated graphene transistors fabricated with these techniques have exceptionally low contact resistances and mobilities which approach theoretical limits.

Second we will present a new strategy for tailoring the stoichiometry of functionalized graphene compounds through the systematic control of the ratio between adatoms. We demonstrate new ternary HFG compounds and reversible switching of material stoichiometry via the sequential exposure of graphene to low energy H plasma and XeF<sub>2</sub> gas. By patterning regions of different functionalization on a single chip, we perform direct comparisons and show spatially controlled tuning of the relative surface properties such as wettability, friction, electronic conductivity and molecular adhesion. Taken together, these studies show that chemical functionalization offers new atomically precise nanofabrication and materials engineering techniques for scalable engineering of circuitry along all three dimensions.

##### 2:20pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-3 Dual-Route Hydrogenation of the Graphene/Ni Interface, *Rosanna Larciprete*, CNR-Institute for Complex Systems, Roma, Italy; *D Lizzit*, Elettra - Sincrotrone Trieste, Trieste, Italy; *M Trioni*, CNR-Institute of Molecular Science and Technologies, Milano, Italy; *P Lacovig*, *L Bignardi*, *S Lizzit*, Elettra - Sincrotrone Trieste, Trieste, Italy; *R Martinazzo*, Università degli Studi di Milano, Milano, Italy

Although the high surface-to-weight ratio would make graphene (Gr) one of the most promising material for hydrogen accumulation, up to now only moderate gravimetric density values of 1-2% have been obtained at room temperature (RT). The ultimate H coverage is limited by the competition between the adsorption and desorption/abstraction processes and by the elastic energy that accumulates in the C lattice once puckered by the local sp<sup>3</sup> hybridization of the C atoms binding hydrogen. Moreover, for epitaxial Gr on metals, the substrate-induced Gr corrugation might modulates periodically H adsorption. In this respect, the Gr/Ni(111) interface appears much more favorable than other graphene/metal systems, as the limitations due to the presence of the moiré supercell vanish due to commensurate relation between the Gr and Ni(111) lattices. Moreover, hydrogenation might be favored by the peculiar reactivity of Gr/Ni(111). This issues motivated a re-investigation of the interaction of this particular interface with hydrogen.

In this study [1] we used x-ray photoelectron spectroscopy (XPS) and near edge x-ray absorption fine structure spectroscopy (NEXAFS) to follow the RT hydrogenation of Gr/Ni(111) and determined the configuration of the hydrogenated interface by scanning tunneling microscopy (STM). We found that hydrogenation proceeds through a dual path that includes hydrogen chemisorption on top of the graphene followed by a slow but continuous intercalation below graphene. At low coverage H atoms predominantly adsorb as monomers and chemisorption saturates when ≈ 25% of the surface is hydrogenated. The formation of C-H bonds determines new

components in the C 1s core level spectrum that are attributed by DFT calculations to C atoms directly bonded to H and to their first neighbors. In parallel with chemisorption, with a much lower rate, H atoms intercalate below Gr and bind to Ni surface sites. Thermal programmed desorption measurements showed that chemisorbed hydrogen is released around 600 K, whereas the intercalated phase desorbs abruptly slightly below 400 K. Then the Gr cover, besides offering a storage volume for the intercalated H, stabilizes it above room temperature rising by a few tens of kelvins the H<sub>2</sub> release temperature with respect to the bare Ni(111) surface.

The effectiveness of these results can be expanded by using Ni substrates with large specific surface, as nanoparticles or nanostructured foils, which, when covered with Gr, might become media where hydrogen can be loaded and stored above room temperature.

[1] D. Lizzit et al. ACS Nano 13 (2019) 1828

##### 2:40pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-4 Assembly of Arrays of Predefined Monolayer Features into vdW Heterostructure by a Continuous Exfoliate-align-Release Process, *Vu Nguyen*, *H Taylor*, University of California at Berkeley

One of the major challenges of van der Waals (vdW) integration of 2D materials is the high-yield and -throughput assembly of pre-defined sequence of monolayers into heterostructure arrays. Although a variety of techniques have been developed to exfoliate the 2D materials from the source and deterministically place them onto a target substrate, they typically can transfer only either a wafer-scale blanket or a small flake at a time with uncontrolled size and shape. Here we present a method to exfoliate arrays of lithographically defined monolayer MoS<sub>2</sub> and WS<sub>2</sub> features from multilayer sources and directly transfer them in a deterministic manner onto target substrates. The continuous exfoliate-align-release process, without the need of an intermediate carrier substrate, was enabled by a new transfer medium fabricated by spin-coating a low-crosslinked and transparent adhesive on a transparent, electrostatically active backing material with low surface energy. MoS<sub>2</sub>/WS<sub>2</sub> vdW heterostructure arrays produced by this method were characterized, showing coupled photoluminescence between the monolayers. Light-emitting devices using WS<sub>2</sub> monolayer were also demonstrated, proving the functionality of the fabricated materials. This method promises to produce large-area monolayer and multiplex heterostructure arrays with capability to integrate with existing semiconductor manufacturing equipment.

##### 3:00pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-5 van der Waals Heterojunction Photothermoelectric Effect in MoS<sub>2</sub>/Graphene Monolayers, *Yunqiu Kelly Luo*, The Ohio State University; *T Zhou*, University at Buffalo, State University of New York; *M Newburger*, The Ohio State University; *R Bailey-Crandell*, *I Lyalin*, The Ohio State University; *M Neupane*, U.S. Army Research Laboratory; *A Matos-Abiague*, Wayne State University; *I Zutic*, University at Buffalo, State University of New York; *R Kawakami*, The Ohio State University

Two-dimensional (2D) van der Waals (vdW) heterostructures provide a vast playground for exploring new phenomena due to its unique ability to tailor and combine dissimilar materials with atomic precision. In particular, the combination of graphene and transition metal dichalcogenides (TMDC) garners immense interest due to their novel optoelectronic, valleytronic and spintronic properties. Here, we report the observation of a highly tunable vdW heterojunction photothermoelectric effect (HPTE) in dual-gated MoS<sub>2</sub>/graphene heterostructures, identified by a signature six-fold photocurrent pattern as a function of heterojunction bias and carrier density. In stark contrast to photovoltaic and photothermionic effects, we discover a new mechanism arising from photoexcitation of hot electrons in graphene and subsequent thermoelectric transport across the vdW junction. While analogous to lateral photothermoelectric effects at quasi-1D junctions in single layers, the vertical geometry of HPTE offers area scaling of 2D active regions and establishes, for the first time, the photothermoelectric response in vdW heterostructures. Operating at both low (18 K) and room temperatures, the discovery of HPTE creates new

possibilities for electrically-tunable broadband photodetectors and atomically-thin spin caloritronic devices.

**3:20pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-6 Formation of Edge-bonded MoS<sub>2</sub>-graphene Nanoribbons by On-surface Synthesis, Mark Hastrup, M Mammen, J Rodríguez-Fernández, J Lauritsen, Aarhus University, Denmark**  
2D materials exhibiting unique material properties have the potential for a huge impact on our future. Graphene, as the first discovered truly 2D material, has been extensively studied. However, the lack of an intrinsic band gap makes it inadequate for electronic and optical devices. MoS<sub>2</sub> from the family of transition metal dichalcogenides has been intensively investigated for its possibility to be used in future applications. The vision is to integrate various 2D materials to realise an actual device. However, the actual assembly of these materials with high controllability remains a challenge. Vertical heterostructures, supported by Van der Waals interactions, have already been realised by manually stacking 2D materials on top of each other[1]. An ultimate thin device can be realised by creating lateral heterostructures with atomically sharp interfaces where each material is directly bonded to another. Currently, methods for in-plane bonding of MoS<sub>2</sub> to other materials (e.g. graphene) are limited due to poor structural match. One possible solution is to develop selective bottom-up methods for synthesis of molecular nanostructures by self-assembly.

This study aim to investigate the fundamental nature of bonding of graphene nanoribbons (GNRs) to the edges of MoS<sub>2</sub> nanoparticles by scanning tunnelling microscopy (STM). The aim is to synthesise GNRs from precursor molecules through a thermally activated Ullmann reaction already used elsewhere[2,3]. After initial growth of MoS<sub>2</sub>, it is necessary to anneal in a hydrogen atmosphere to activate the edges to facilitate the attachment of an intermediate structure of poly(para-phenylene) (PPP) wires. STM reveals the PPP wires have an affinity for the corners of the MoS<sub>2</sub> nanoparticles with a distance, obtained from line scans across the adsorption site, consistent with a covalent C-S bond.

[1]: Pant et al., *Nanoscale*, 2016, 8, 7, 3870-3887

[2]: Cai et al., *Nature*, 2010, 466, 7305, 470-473

[3]: Basagni et al., *J. Am. Chem. Soc.*, 2015, 137, 5, 1802-1808

**4:00pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-8 The Effects of Metal-modification and Two Dimensional (2D) Lamellar Structure on Catalytic Performance of MFI Zeolite for Ethylene Conversion into Liquid Aromatics, Laleh Emdadi, L Mahoney, D Tran, I Lee, US Army Research Laboratory**

The effects of two dimensional (2D) meso-/microporous structure and metal modification with gallium or zinc on catalytic performances of lamellar MFI zeolites in ethylene conversion reaction to liquid aromatics were investigated. Dual template technique was used to synthesize the 2D zeolite and metal modification of the zeolite was carried out by wet impregnation method. The results of multiple analysis techniques such as TEM, XRD, Ar adsorption-desorption, UV-Visible spectroscopy, and H<sub>2</sub>-TPR showed that the zeolite structure is a pivotal factor for controlling the type of metal dopant species forming on zeolite, their size, and their distribution. Adding metal dopants to 2D zeolite structures improved the yield of liquid aromatics and selectivity for mono-benzene alkylated aromatics compared to their microporous commercial MFI analogies while decreased the coke formation rate. Zinc loaded lamellar MFI had the most efficient catalytic performance among all studied catalysts with lowest amount of total coke and highest fraction of light coke including mono-benzene alkylated aromatics determined by combination of different techniques such as FTIR, UV-Vis, MS-temperature programmed oxidation (TPO), FTIR-TPO, and GC-MS. This can be explained by higher accessibility of reactants to active sites and facilitated transport of products and coke precursors from lamellar structure of this zeolite and the lower Brønsted/Lewis acid site ratio of this catalyst provided by metal modification which is more suitable for ethylene aromatization and suppresses the formation of heavy coke species. The catalytic performance of zeolite catalyst can be tuned by modulating both the textural and acidity properties of the zeolite structure. The metal modified 2D lamellar MFI zeolites as bifunctional catalysts open an avenue for converting large reactant molecules to desired products by designing a catalyst with an optimal structure, acidity, and dispersion of metal dopants.

**4:20pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-9 Structural Stability of Graphene Nanoflakes:From the View Point of Aromaticity, M Ushirozako, H Matsuyama, A Akaishi, Jun Nakamura, The University of Electro-Communications (UEC-Tokyo), Japan**

Recently, nano-scale graphene nanoflakes (GNFs) have attracted great attention as one of the promising materials for electronics and spintronics. Kim *et al.* have successfully fabricated GNFs with various sizes up to 35 nm and have reported that the photoluminescence property of GNFs depends on the size and the edge shape [1]. From the view point of the structural stability of GNFs, we have not yet acquired the systematic comprehension with regard to effects of shapes and sizes of GNFs on the stability. In the present study, we have examined how the stability of GNFs is dominated by the edge shape and the size of GNFs, using first-principles calculations within the density functional theory.

In order to evaluate the stability of GNFs, we calculated the edge formation energy. First, we consider GNFs with the six-fold symmetry (D<sub>6h</sub>) and classify them into zigzag GNFs (ZZGNFs) and armchair GNFs (ACGNFs). ACGNFs have two subtypes, AC(1) and AC(2), depending on whether carbon atoms are just at the corner of the outermost envelope hexagon of GNFs. We define the edge purity as the ratio of the number of carbon atoms at the edge unambiguously regarded as the armchair to the total number of edge atoms. The purity of AC(1) is higher than that of AC(2). The chemical formulae associated with ZZ, AC(1), and AC(2) are C<sub>6n</sub><sup>2</sup>H<sub>6n</sub>, C<sub>18n</sub><sup>2-18n+6</sup>H<sub>12n-6</sub>, C<sub>18n</sub><sup>2-30n+12</sup>H<sub>12n-12</sub>, respectively. In addition, we also evaluate the structural stabilities of triangular and rhombus GNFs.

We calculated the edge formation energy of the GNFs having up to 1200 carbon atoms as a function of the number of edge carbon atoms [3]. The formation energy of ZZGNFs is higher than that of ACGNFs irrespective of the size of GNFs. This instability of ZZGNFs is attributed to the presence of the so-called edge state. Indeed, it has also been shown that the formation energy of the zigzag graphene nanoribbon is higher than that of the armchair one [4]. It is noted that AC(2) is slightly more stable than AC(1), whereas the purity of AC(2) is lower than that of AC(1). Such peculiar stabilization can be reasonably explained in terms of the aromaticity of GNFs. The Nucleus Independent Chemical Shifts (NICS) values, which is averaged for the six-membered rings in GNFs, for AC(2) are lower than those for AC(1). This means AC(2) is more aromatic than AC(1). We will discuss the quantitative relationship between the stability and the aromaticity of GNFs.

[1] S. Kim et al., *ACS Nano*, 6, 9, 8203 (2012)

[2] W. Hu *et al.*, *J. Chem. Phys.* 141, 214704 (2014)

[3] A. Akaishi, M. Ushirozako, H.Matsuyama, and J.Nakamura, *Jpn.J.Appl.Phys.* 57, 0102BA(2018)

[4] S. Okada. *Phys. Rev. B*, 77, 041408 (2008)

**4:40pm 2D+AP+EM+MI+MN+NS+PS+TF-MoA-10 Wafer-scale 2D-3D Mixed Heterostructures Enabled by Remote Epitaxy through Graphene, Jeehwan Kim, Massachusetts Institute of Technology**  
**INVITED**

The current electronics industry has been completely dominated by Si-based devices due to its exceptionally low materials cost. However, demand for non-Si electronics is becoming substantially high because current/next generation electronics requires novel functionalities that can never be achieved by Si-based materials. Unfortunately, the extremely high cost of non-Si semiconductor materials prohibits the progress in this field. Recently our team has invented a new crystalline growth concept, termed as "remote epitaxy", which can copy/paste crystalline information of the wafer remotely through graphene, thus generating single-crystalline films on graphene [1,2]. These single-crystalline films are easily released from the slippery graphene surface and the graphene-coated substrates can be infinitely reused to generate single-crystalline films. Thus, the remote epitaxy technique can cost-efficiently produce freestanding single-crystalline films including III-V, III-N, and complex oxides. This allows unprecedented functionality of flexible device functionality required for current ubiquitous electronics. I will also present detailed mechanism behind remote atomic interaction through graphene [2]. In addition, we have recently demonstrated a manufacturing method to manipulate wafer-scale 2D materials with atomic precision to form monolayer-by-monolayer stacks of wafer-scale 2D material heterostructures [3]. In this talk, I will discuss the implication of this new technology for revolutionary design of next generation electronic/photonic devices with combination of 3D/2D mixed heterostructures.



# Monday Afternoon, October 21, 2019

[1] Y. Kim, et al, and J. Kim, "Remote epitaxy through graphene enables two-dimensional material based layer transfer" *Nature*, Vol. 544, 340 (2017)

[2] W. Kong, et al, and J. Kim, "Polarity govern atomic interaction through two-dimensional materials", *Nature Materials*, Vol. 17, 999 (2018)

[3] J. Shim, S. Bae, et al, and J. Kim, "Controlled crack propagation for atomic precision handling of wafer-scale two-dimensional materials" *Science*, 362, 665 (2018)

## MEMS and NEMS Group

### Room A210 - Session MN-MoA

#### Microfabricated Systems for Gas Chromatography and Nanomechanical Mass Sensing

**Moderators:** Robert Davis, Brigham Young University, Christian Zorman, Case Western Reserve University

#### 1:40pm MN-MoA-1 Micromachined Silicon Micro-pillar Arrays for Liquid and Gas Chromatography, *Gert Desmet*, Vrije Universiteit Brussel, Belgium **INVITED**

The present contribution aims at illustrating and demonstrating how micro-machining technology can give a boost to High Performance Liquid Chromatography (HPLC). Currently, HPLC is routinely used in nearly every chemical analysis lab. Despite its high degree of maturity, the technique however suffers from serious performance limitations when faced to the complex samples that need to be separated to solve the current state-of-the-art problems in the biological and pharmaceutical research (e.g., proteomics and metabolomics), the food and environmental analysis, etc.

The currently used packed bed HPLC columns are clearly underachieving because of the packing disorder and the concomitant large degree of band broadening. To solve this packing disorder problem, the present contribution will focus on the possibilities of advanced photolithographic etching techniques such as the Bosch-process to produce perfectly ordered porous support columns with optimized hydrodynamic shape and optimized external porosity.

At the conference, we will demonstrate the possibility of rapid multi-component separations and the possibility to achieve very high separation efficiencies with a microfabricated column in pressure-driven liquid chromatography. In addition, we have also extended the concept to gas chromatography (GC), where the micromachining allows to make designs that combine fast separation kinetics with a high mass loadability, two factors with opposite requirements in the current commercial format for GC.

#### 2:20pm MN-MoA-3 An Integrated Passive $\mu$ Preconcentrator with Progressively-Heated $\mu$ injector for $\mu$ GC, *R Hower, C Zhan, M Akbar, N Nuñovero, J Wang, J Potkay, Edward Zellers*, University of Michigan **INVITED**

We report on a new device designed to serve as a universal 'front-end' for gas chromatographic microsystems ( $\mu$ GC) for remote, long-term monitoring of vapor-phase chemical threats or environmental pollution. This small, low-power, Si/glass-micromachined device, dubbed a micro-collector/injector ( $\mu$ COIN), combines a passive micro-preconcentrator ( $\mu$ PP) with a progressively heated micro-injector ( $\mu$ PHI). The  $\mu$ PP samples vapors at known rates by molecular diffusion and transfers them under active flow via thermal desorption to the  $\mu$ PHI, which, in turn, injects them to a downstream ( $\mu$ GC) separation column via progressive (sequential) heating. Most testing to date was performed with discrete devices, both of which contain tandem cavities packed with granular carbon-based adsorbents of different specific surface areas. Carboxen B (CB, 100 m<sup>2</sup>/g) and Carboxen X (CX, 240 m<sup>2</sup>/g) were used for most compounds. But CX was used with Carboxen 1003 (C3, 1000 m<sup>2</sup>/g) for more volatile compounds. Using a conventional GC for downstream analyses, we have found that the  $\mu$ PP (CX/CB) can collect vapors of widely different volatility at a nearly constant effective sampling rate for up to 24 hrs (low concentrations) and over a 2,500-fold concentration range (0.25-hr samples). Effective (compound-specific) sampling rates ranged from ~0.25 to 0.69 mL/min, most of which agreed with theoretical predictions. Desorption/transfer efficiencies from the  $\mu$ PP were > 87% (most > 94%) at 5 mL/min and 250 °C for 60 sec. For the  $\mu$ PHI (CX/CB) bolus challenges of compounds at 5mL/min, mimicking transfer from the  $\mu$ PP, resulted in > 90% capture efficiency for up to 3.6  $\mu$ g of lower volatility compounds. More volatile or highly polar compounds required the CX/C3-loaded device. Back-

flushed progressive heating of the  $\mu$ PHI produced injection bands < 250 ms wide at flow rates < 0.5 mL/min. In separate tests, remarkable selectivity for polar compounds was achieved by applying an ionic-liquid surface modifier to the carbon adsorbents (tests in the  $\mu$ PP and  $\mu$ PHI are pending). The monolithically integrated  $\mu$ COIN (0.23 cm<sup>3</sup>) has not yet been tested. But, a hybrid-integrated  $\mu$ COIN (capillary connections) provided good preliminary performance, including efficient sampling, transfer, and injection of multi-component mixtures. Valveless flow modulation was implemented to avoid backflow to the  $\mu$ PP. Using typical power levels for each device, two valves, a pump, an interconnect heater, and supporting electronics, the energy consumption was only 320 J per cycle for the hybrid  $\mu$ COIN. Thus, the  $\mu$ COIN shows promise as a component in future ultra-low-power  $\mu$ GC systems for analyzing complex vapor mixtures.

#### 3:00pm MN-MoA-5 Developments and Challenges in Full-range Microchip Gas Chromatography, *Abhijit Ghosh*, Honeywell UOP, Des Plaines, IL, USA.; *M Lee*, Brigham Young University

This year (2019) marks the 40th anniversary of microchip gas chromatography (GC). In these four decades of investigations, many avenues, as well as challenges, have been encountered by researchers to produce microchip columns that are as efficient as fused silica open tubular columns in GC. Although there are exciting theoretical possibilities, in reality many practical constraints remain that limit their widespread commercialization and use. The main challenges are difficulty in static coating, unwanted dead volumes and inadequate interfacing technologies, which all affect both column performance and range of applications. This presentation emphasizes some of the challenges and key developments in the field of microchip gas chromatography, as well as novel approaches that are currently being investigated

#### 3:20pm MN-MoA-6 Fabrication of Thermally Isolated micro-Column for Gas Chromatography, *James Harkness, H Davis, A Davis, R Davis, B Jensen, R Vanfleet*, Brigham Young University

Micro gas chromatography (GC) has suffered from poor separations due to short column length and stationary phase pooling, however introducing a thermal gradient along a GC micro-column has been shown to enhance separations. We will present a thermally isolated micro-column for thermal gradient GC, fabricated using a two-wafer deep silicon etch/bond/etch process. Desired thermal isolation was achieved by forming suspended micro-columns that enable low-power thermal control using passive and active elements.

#### 4:00pm MN-MoA-8 Control of Surface Geometry and Chemistry to enable integration of Microfabricated Structures into High Performance Microscale Gas Chromatography Systems, *Henry Davis, D McKenna, J Harkness, D Kane, R Vanfleet, R Davis*, Brigham Young University

There are a variety of microfabricated structures, materials and devices that could enable high performance microscale gas chromatography systems, such as micro pillar arrays and porous resonant mass detectors. However, integration of these structures into microscale gas chromatography systems will require a high degree of control over surface geometry and surface chemical functionalization. Here we will describe processes using liquid deposition of silsesquioxanes and oxide atomic layer deposition for control of surface chemistry and geometry of micro and nanoscale structures.

#### 4:20pm MN-MoA-9 Constructive Utilization of Nonlinear Dynamics in MEMS/NEMS, *Hanna Cho*, The Ohio State University **INVITED**

During the last decades, we have witnessed that MEMS/NEMS revolutionized fundamental and applied science. However, due to small size and low damping, these devices often exhibit significant nonlinearity and thus the operational range of these impressive applications shrinks. Therefore, understanding the mechanisms leading to nonlinearity in such systems will eliminate obstacles to their further development and significantly enhance their performance. Motivated by the need to advance current capabilities of MEMS/NEMS, our research has been focused on the implementation of intentional intrinsic nonlinearity in the design of MEMS/NEMS resonators and proved that harnessing intentional strong nonlinearity enables exploiting various nonlinear phenomena, not attainable in linear settings, such as broadband resonances, dynamic instabilities, nonlinear hysteresis, and passive targeted energy transfers. We developed a comprehensive analytical, numerical, and experimental methodology to consider structural nonlinearity as a main design factor enabling to tailor mechanical resonances and achieve targeted performance. We investigated the mechanism of geometric nonlinearity in a non-prismatic microresonator and suggested strategies to tailor the

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various types of nonlinear resonance. Our recent works focus on exploiting nonlinearity and multimodality simultaneously by internally coupling two or more modes through the mechanism of internal resonance or combination resonance. This talk will introduce various types of nonlinearity realized in micro/nanomechanical systems and discuss their unique behavioral features that can be exploited in the field of MEMS/NEMS.

**5:00pm MN-MoA-11 Frequency Stabilization in a MEMS Oscillator Via Tunable Internal Resonance, Jun Yu, H Cho, The Ohio State University**  
Micro-Electro-Mechanical Systems (MEMS) oscillators are being considered as substitutes of quartz oscillators since these microscale oscillators are easier to be integrated in electronics. As a timing device, one of the most important functionalities of MEMS oscillators is to provide a reference frequency with a minimal frequency fluctuation. The mechanism of internal resonance (IR) was proposed to stabilize the frequency by Antonio et al. in 2012 [1]. Here, we report a MEMS resonator that is specifically optimized to provide 1:2 relationship between its modal frequencies and, thus, implement 1:2 IR in its dynamic response. We also tune the frequency ratio precisely by adjusting the applied DC voltage to achieve an ideal IR characteristic for frequency stabilization.

In this study, a clamped-clamped silicon microbeam resonator shown was designed and fabricated to enforce a 1:2 ratio between its second and third flexural modes. We first characterized the thermal-mechanical noise of the resonator under different DC biases using a Laser Doppler Vibrometer. Its modal frequencies can be tuned with DC bias, because the DC bias influences the mid-plane stretching of the microbeam structure. Thereby, the ratio between second and third flexural modes can be finely adjusted around the 1:2 commensurate condition and eventually achieve exact 1:2 ratio when the DC bias is 21V. Under this IR condition, a well-documented M-shape, typically occurring in a 1:2 IR system. The externally resonated (ER) curve represents the oscillation amplitude at the excitation frequency, while the internally resonated (IR) curve represents the oscillation amplitude at the twice of the excitation frequency. We further studied the frequency stabilization by exploiting the energy transfer mechanism of internal resonance. We measured the frequency fluctuations from the MEMS oscillator implementing this resonator in the cases without and with IR. When IR was triggered, the frequency fluctuation was diminished by more than 20 times to be 5.72 ppm. The Allan deviations is also reduced by about 30 times when the IR is activated.

[1] D. Antonio, D. H. Zanette, and D. López, "Frequency stabilization in nonlinear micromechanical oscillators," *Nat. Commun.*, vol. 3, no. 1, Jan. 2012.

## 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 Mariani, University of Waterloo, Canada; C Earnest, University of 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  $\sim 10$  nm Si layer, followed by a thin  $\sim 1$  nm SiGe layer, and subsequent  $\sim 2$  nm layer of pure Si. Above this quantum well, a  $\sim 35$  nm layer of SiGe with 29% Ge is grown to separate the quantum well from the surface. The intent of this  $\sim 1$  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  $100,000 \text{ cm}^2/(\text{V s})$  at  $6 \times 10^{11} \text{ cm}^{-2}$  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  $\mu\text{eV}$ , 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 Filippi, 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, a 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-Abiad, 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

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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 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<sup>th</sup> 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  $\text{TiSe}_2$ ,  $\text{TiTe}_2$ , and  $\text{VSe}_2$ . 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  $\text{TiSe}_2$ , we observe an orbital-selective CDW, necessarily without a  $k_z$ -selectivity in band hybridisation that is of key importance for the bulk instability,<sup>1</sup> while  $\text{TiTe}_2$  is driven into a charge-ordered phase in the monolayer which is not stable in the bulk at all. In  $\text{VSe}_2$ , 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.<sup>2</sup> 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.*

<sup>1</sup>Watson *et al.*, Phys. Rev. Lett. 122 (2019) 076404.

<sup>2</sup>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  $\text{MoSe}_2/\text{WSe}_2$  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  $\text{MoSe}_2/\text{WSe}_2$  hetero-bilayer encapsulated in h-BN with the alignment angle close to 60 degree between  $\text{MoSe}_2$  and  $\text{WSe}_2$ . 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. *Ab 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* electronic transitions. These peaks are *double indirect* 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<sub>2</sub> with Topological Insulator Bi<sub>2</sub>Se<sub>3</sub>**, *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<sub>2</sub>Se<sub>3</sub>. Monolayer of MnSe is grown on Bi<sub>2</sub>Se<sub>3</sub> 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<sub>2</sub> on Bi<sub>2</sub>Se<sub>3</sub> surface. By performing spin-polarized STM measurement with Cr tip, we observed directly the magnetic signal from 1T-MnSe<sub>2</sub> on Bi<sub>2</sub>Se<sub>3</sub>. The growth of 1T-MnSe<sub>2</sub> on Bi<sub>2</sub>Se<sub>3</sub> further leads to the MBE synthesis of magnetic topological insulator Bi<sub>2</sub>MnSe<sub>4</sub>, 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.

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2. M. Mehboudi, et al., *Phys. Rev. Lett.* **117**, 246802 (2016).
3. S. Barraza-Lopez, et al., *PRB* **97**, 024110 (2018).
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11:00am **2D+EM+MI+MN+NS+QS-TuM-10 Sign-change Pairing Symmetry in Single Layer FeSe/SrTiO<sub>3</sub> 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<sub>3</sub>(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 pairing 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<sub>3</sub> 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<sub>3</sub> 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<sub>1-x</sub>Se<sub>x</sub>/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<sub>1-x</sub>Se<sub>x</sub> down to the single atomic layer limit. High quality single layer FeTe<sub>1-x</sub>Se<sub>x</sub> films are grown on SrTiO<sub>3</sub>(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  $\Gamma$  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  $\Gamma$  point. For  $x > 0.1$ , the hole pocket at  $\Gamma$  point moves below the Fermi level, and an electron-pocket emerges at M point where a superconducting gap opens with a  $T_c$  of  $\sim 50$  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<sub>0.55</sub>Se<sub>0.45</sub>, 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<sub>0.55</sub>Se<sub>0.45</sub> 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<sub>0.55</sub>Se<sub>0.45</sub> 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  
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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<sup>1,2</sup>, L.Y. Kong<sup>1,2</sup>, P. Fan<sup>1,2</sup>, H. Chen<sup>1</sup>, S.Y. Zhu<sup>1,2</sup>, W.Y. Liu<sup>1,2</sup>, L. Cao<sup>1,2</sup>, Y.J. Sun<sup>1,2</sup>, S.X. Du<sup>1,2,3</sup>, J. Schneeloch<sup>4</sup>, R.D. Zhong<sup>4</sup>, G.D. Gu<sup>4</sup>, Liang Fu<sup>5</sup>, Hong Ding<sup>1,2,3</sup>.

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## MEMS and NEMS Group Room A210 - Session MN-TuM

### MEMS, BioMEMS, and MEMS For Energy: Processes, Materials, and Devices II

**Moderators:** Robert Davis, Brigham Young University, Zenghui Wang, Case Western Reserve University

8:00am **MN-TuM-1 Near-Zero Power Integrated Microsystems for the IoT**, *Matteo Rinaldi*, Northeastern University  
**INVITED**

The recent advancements in terms of sensor miniaturization, low power consumption and low cost allow envisioning a new era for sensing in which the data collected from multiple individual smart sensor systems are combined to get information about the environment that is more accurate and reliable than the individual sensor data. By leveraging such sensor fusion, it will be possible to acquire complete and accurate information about the context in which human beings live, which has huge potential for the development of the Internet of Things (IoT). To address the growing demand of such large wireless sensor networks, there is a need for wireless sensors with dimensions and power consumption that are orders of magnitude smaller than the state-of-the-art. Energy is the key challenge. Batteries have limited capacity, and existing sensors are not "smart" enough to identify targets of interest. Therefore, they consume power continuously to monitor the environment even when there is no relevant data to be detected. This talk presents a new class of zero-power microsystems that fundamentally brake this paradigm, remaining dormant, with zero-power consumption, until awakened by a specific physical signature associated with an event of interest. In particular, a zero-power infrared (IR) digitizing sensor microsystem consisting of plasmonically-enhanced micromechanical photoswitches is presented. Such a passive IR digitizer is capable of producing a wake-up bit when exposed to a specific IR spectral signature associated to a target of interest (such as the exhaust plume of a car, a forest fire, or a human body) while rejecting background interference. The capability of these zero-power sensors of consuming power only when useful information is present results in a nearly unlimited duration of operation, with a groundbreaking impact on the proliferation of the IoT.

8:40am **MN-TuM-3 Development of Inorganic Metal Salt Inks for Printable Sensor Applications**, *Y Sui*, Case Western Reserve University; *A Hess-Dunning*, Louis Stokes Cleveland VA Medical Center; *M Sankaran*, *Christian Zorman*, Case Western Reserve University

The rapid advancement of flexible and stretchable electronics has stimulated the development of printing approaches as a means to fabricate metallic interconnects, antenna and other essential conducting structures. Unfortunately, metal inks have been limited to silver, copper, and gold, due to the complexity of nanoparticle synthesis and metallo-organic compound design. While sufficient for interconnects, the development of printed sensors is significantly limited by the small selection of printable metals. Recently, we reported a new class of inks that are based on inorganic metal salts that are converted to metallic structures by exposure to a low-

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temperature inert gas plasma. This approach to ink design opens up a much wider range of printable metals than currently available from conventional inks. We found that chemical, biological and mechanical sensors fabricated using this printing approach significantly outperformed the same sensors fabricated using conventional approaches, presumably due to the surface morphology of the printed sensors.

In this paper, we describe a method of controlling the surface morphology for metal structures fabricated using plasma activation of inorganic metal salt-based inks. We have found that the ink solvent plays a key role in the nucleation and crystal growth of metal nanostructures during the plasma reduction process. Using solvents of different vapor pressures, we were able to control the duration of plasma-induced liquid-phase nucleation and crystallization, thereby tuning the surface morphology, conversion depth, and resistivity of the printed metal structures. Silver nitrate-based ink was used for this study and the ink solvents in order of decreasing vapor pressure were ethylene glycol (EG), di-ethylene glycol (di-EG), and tri-ethylene glycol (tri-EG). The structural, morphological, and electrical properties of metals printed with different ink solvents were characterized by cross-sectional scanning electron microscopy (SEM), optical profilometry, and sheet resistance measurements, respectively. To show that the tunable morphology can be used to enhance the sensitivity of printed sensors, we fabricated and tested a silver-based hydrogen peroxide sensor using inks made from the three solvents.

**9:00am MN-TuM-4 Void-Free Copper Electrodeposition in Full Wafer Thickness Through-Silicon Vias with 10:1 Aspect Ratios, Rebecca Schmitt, L Menk, C Sadler, E Baca, A Hollowell, Sandia National Laboratories**

Copper-filled through-silicon vias (TSVs) are incorporated in microelectronic devices as a 3D integration technique to increase I/O per unit volume. Industry has incentivized thinning wafers to increase TSV density, but certain MEMS applications require full thickness substrates, thus creating a demand for mesoscale TSVs. Using a full thickness silicon wafer helps preserve wafer flatness during multi-layer device fabrication and conserves mass, often required in MEMS applications. Traditionally, a three-additive Cu deposition chemistry is used for TSV filling; however, in this work, a single-additive chemistry has been established to achieve bottom-up superfilling in high-aspect ratio features. This electroplating chemistry involves a mixture of  $\text{CuSO}_4$ ,  $\text{CH}_3\text{O}_3\text{S}$  or  $\text{H}_2\text{SO}_4$ , chloride, and a poloxamine suppressor additive. Cyclic voltammetry (CV) can be used to characterize the electrolyte and identify a hysteretic region, which is caused by suppressor breakdown at the cathode surface. This hysteresis corresponds to an operating window where void-free Cu filling of high-aspect ratio features can be achieved.

Previously, potentiostatic and galvanostatic deposition conditions for void-free filling were developed for nominally 100  $\mu\text{m}$  diameter and 600  $\mu\text{m}$  deep vias. Copper electrodeposition in TSVs with a 10:1 aspect ratio is currently under investigation. These TSVs have a 62.5  $\mu\text{m}$  diameter etched into a 625  $\mu\text{m}$  thick silicon-on-insulator (SOI) wafer. However, the conditions that resulted in void-free, bottom-up filling in 100  $\mu\text{m}$  diameter TSVs have not translated to fill 62.5  $\mu\text{m}$  geometries. In this work, electrolyte constituent concentrations, applied potential, and applied current were varied to analyze their effect on fill profile in 62.5  $\mu\text{m}$  TSVs. Fill profiles were analyzed through cross sectioning and optical microscopy, as well as through X-ray CT scans. This work details the experimental approach associated with determining electrodeposition conditions for 62.5  $\mu\text{m}$  diameter TSVs and presents the resulting fill profiles of copper in these vias.

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**9:20am MN-TuM-5 Ion-Conducting Materials and Devices for Cold Atom Microsystems, Christopher Roper, HRL Laboratories, LLC; S Kang, NIST; R Matt, A Mis, HRL Laboratories, LLC; E Donley, J Kitching, NIST**

Atomic instruments using laser-cooled atoms in ultra-high vacuum enable highly precise measurements of time, acceleration, and rotation [1]. Use of such devices outside the laboratory requires control of the atomic vapor density to prevent warm atoms from prematurely disturbing the cold atoms prior to measurement. Portable, miniature cold atom devices require a low-power, scalable method for controlling atomic vapor density.

Recently, solid-state electrochemical devices based on the solid electrolyte beta"-alumina have been used to change Rb vapor density on the scale of first 100s [2] and then 10s [3] of seconds. Reduction in vapor density up to

7X has been reported. Furthermore, these devices have been used to stabilize Rb vapor density using a feedback loop [4].

We present a solid-state electrochemical device consisting of a fine Pt grid top-electrode with submicron lithographically patterned features, beta"-alumina solid electrolyte, patterned Pt bottom electrode, and graphite reservoir. For relatively slow actuation cycle frequencies (17 mHz), this device exhibits a 100X increase in Rb vapor density with -30 V sourcing voltage and 20X decrease in the Rb vapor density with +30V sinking voltage. Rb vapor density can be modulated at up to 50 Hz, although at lower Rb vapor density dynamic range. An inverse relationship is found between Rb vapor density dynamic range and actuation cycle frequency. The high vapor density dynamic range and fast cycling rates demonstrated with this device are attributed to the fine, submicron top electrode features compared to coarse top electrode features (>100  $\mu\text{m}$ ) used in prior works. These devices are expected to be key components in future cold atom microsystems.

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**9:40am MN-TuM-6 Determining the Material Properties of Carbon Nanotube Structures Through Cantilever Resonances, Richard Cass, Brigham Young University; E Eion Hindsman-Curry, University of Alabama; R Vanfleet, R Davis, D Alfred, B Anderson, R Vanfleet, Brigham Young University**

Nanotube Templated Microfabrication (CNT-M) processes use nanotube forest growth from a 2-D pattern to form 3-D structures. The resulting structure is then infiltrated with a second material to form the final device. Materials properties of these structures with different infiltration materials and varying degrees of infiltration is of interest.

We have used force-displacement data (in fixed-free and 3-point bending configurations) to determine the Ultimate Strength, the Young's Modulus, and the Maximum Strain of CNT-M structures using various infiltration materials. However, in the case of tungsten infiltration processes and typical test beams (~250  $\mu\text{m}$  in width), the infiltration was not sufficiently uniform for high confidence results. Smaller beams (< 50  $\mu\text{m}$  width) are difficult to handle using the conventional 3-point bending processes. We report resonance frequency testing, using a Laser Doppler Vibrometer (LDV), of thin CNT-M cantilevers to find the Young's Modulus of these CNT structures.

**11:00am MN-TuM-10 Nanoporous Titanium Nitride Electrodes for Biosensing, Mark Ming-Cheng Cheng, G Chen, Wayne State University**

We report corrosion-resistant and high-capacity implantable nanoporous titanium nitride (TiN) electrodes for neural probes applications. Traditionally, the TiN electrodes are prepared using reactive sputtering techniques and have limited surface areas. To research smaller electrodes to minimize tissue damage, high aspect ratio TiN nanotube structures were fabricated using electrochemical anodization of Ti wires followed by high-temperature nitration. The specific charge capacity of nanoporous TiN correlates proportional with the surface area and pore size.

According to Shannon criteria, an empirical rule in neural engineering for possibility of tissue damage from electrical stimulation, the recommended limit density of a stimulation pulse is  $30\mu\text{Ccm}^{-2}$  for a geometric surface area of  $0.06\text{cm}^2$ . Nevertheless, the charge injection capacity of chronically implanted electrodes has shown degraded over the time (within one month to a year), including sputtered iridium oxide (SIROF), porous platinum and tungsten. One of the challenges for these implantable electrodes involves irreversible reduction and oxidation reactions occurring at the electrode surface through faradic or pseudocapacitive charge transfer. On the other hand, TiN has different mechanism of charge injection (through capacitive double layers). TiN has been shown promising electrode material in neural implants thanks to its super electrical conductivity, biocompatibility and chemical stability. TiN is also known for

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physiologically inert and corrosion resistant. To increase the spatial resolution of neural stimulation, small electrodes with high surface areas are more desirable. To the best of our knowledge, TiN nanotubes electrodes have not been studied in the literature for neural implants. Compared to tungsten electrode, the impedance and morphology of nanoporous TiN was found stable over a long-term in stress tests (at an elevated temperatures in phosphorous buffered solution).

11:20am **MN-TuM-11 Toward a Simple Process for Fabricating Multi-channel Neural Probes on Optical Fiber Substrates**, *Md Ashiqur Khan, M Gheewala, V Jonnalagadda, T Tisa, M Rao, A Awale, P Motwani, N Randhawa, H Sajedi, W Shih, J Wolfe*, University of Houston; *J Dani*, University of Pennsylvania; *P Mauger*, No Matching Affiliation

Electrical probes are used to stimulate spiking activity within a target population of neurons and monitor how these electrical signals propagate through the brain. This paper describes a simple fabrication process for multi-electrode neural probes on optical fiber substrates. It relies on neutral particle proximity lithography to achieve the required depth-of-field and freedom from charging artifacts but circumvents the complexity of membrane masks (complementary exposures, radiation resistant coatings, and fragility) and on-fiber alignment.

Fig. 1 of the supplementary document shows, conceptually, a probe with 4-channel thin-film sensor, a tetrode, on each of four sides of a fiber. It requires two masks; the first for the interconnect traces. The other for vias in the dielectric overcoat where the metal lines contact the brain.

As shown in Fig. 2, optical fibers are held in V-grooves etched into the top surface of a (100) Si wafer. A second set of V-grooves, etched from the opposite side of the wafer, forms open windows at the bottom of the upper grooves. When this mask is illuminated by 50 keV He atoms, transmitted beamlets transfer the stencil pattern to resist on the fibers. A negative-tone, plasma-deposited, resist is used to mask the gold interconnects. The vias are similar, but require a tone-reversal step. Rotational alignment of the 2 masks uses a high precision cubic bead glued to the end of the fiber to reference the rotational angle of the fibers to a precision-ground aluminum platform on the jig. Longitudinal alignment is achieved using a fiber-stop. These are high precision (Grade 5) 440C stainless steel ball bearings which are held in an anisotropically etched pocket at the tip-end of a V-groove by a rare earth magnet. Longitudinal and transverse positional errors of  $1.0 \pm 0.6$  mm and  $0.3 \pm 0.15$  mm, respectively. A single-interconnect mask can be printed multiple times to build the probe of Fig.1. The offset is produced by tilting the mask relative to the beam. Fig. 3 shows two lines printed on a 300 mm fiber with 21.5 and 29.5 mm offsets in the longitudinal and transverse directions, respectively.

Fig. 4 is an in-vitro recording from a brain slice (mouse) after a battery of bench tests, including a) a 3-week soak phosphate buffered, b) repeated insertion in agar and a stainless steel cannula, d) disinfection in MetriCide-2.6% glutaraldehyde, and a 6 hour implantation in mouse brain). Impedance spectra were the same within the measurement error of the impedance bridge before and after these bench tests.

At this time the tone reversal process has not been fully optimized.

11:40am **MN-TuM-12 A Low-Temperature Packaging Process for Mechanically-Adaptive Neural Interfaces for Microfluidic-Aided Drug Delivery**, *E Szabo, L Greenwood*, Case Western Reserve University; *Allison Hess-Dunning*, Louis Stokes Cleveland VA Medical Center

Advances in polymer-based materials development have led to an array of environmentally-responsive materials that are uniquely suited for biomedical implant applications. Compatible microfabrication processes continue to be developed to integrate these responsive materials into biomedical microdevices. Progressing beyond proof-of-concept devices into functional implants for long-term use requires additional development of compatible and reliable packaging strategies to facilitate interfacing the microdevices with peripheral components. Our group has previously developed a mechanically-adaptive, polymer nanocomposite-based (NC) intracortical implant with a microfluidic channel for diffusion-based drug delivery. Interfacing the device with fluid pumps requires a means for secure attachment of polyethylene tubing to the inlet and outlet ports of the neural microdevice that will remain stable under physiological conditions. Packaging process considerations include incompatibilities of NC with organic solvents and temperatures exceeding 80°C. Additionally, out-of-plane forces on the devices must be minimized in order to maintain the integrity of the microfluidic channels.

We designed connectors to interface polyethylene tubing with the NC-based neural microdevices, to be built using a multi-jet 3D printer. Components produced using multi-jet printers typically have a plastic structural material and a wax-based support material that is removed during post-processing operations. However, our approach involves using a controlled, thin layer of the wax support material as a functional adhesive between the plastic connector and the NC device. With a melting point of 60°C, the wax is stable at body temperature (37°C) and can be melted and reformed at temperatures below the processing limit for the device. Because the wax is printed as part of the connector, the tubing ports can be aligned to the microfluidic inlet and outlet in a single step. Through this approach, we established a leak-free connector design and packaging process to facilitate a fluidic connection between syringe or osmotic pumps and NC-based microdevices. The adhesive bonding strength provided by the wax to the NC exceeded 37 MPa, much higher than the 0.75 MPa required to pump fluid through the connector and microfluidic channel. Packaged devices remained functional in phosphate buffered saline heated to 37°C, even after soaking for 24 hours. The potential for scaling the packaging process and for applying to other materials will also be discussed.

12:00pm **MN-TuM-13 Vascular Graft Pressure-Flow Monitoring Using Nanocomposite Carbon Black/PDMS Based Strain Sensors**, *Hao Chong*, Case Western Reserve University; *S Majerus*, Louis Stokes Cleveland VA Medical Center; *J Liu, C Zorman*, Case Western Reserve University

A vascular graft is commonly used to bypass damaged blood vessels or to form an arteriovenous shunt for vascular access (e.g. for hemodialysis). Real-time monitoring of blood flow in synthetic grafts would provide early warning of graft failure to permit interventions such as angioplasty or graft replacement to avoid catastrophic failure. Based on biocompatible materials, we have developed a new type of flexible pulsation sensor (FPS) which is wrapped around a graft to monitor blood pressure and flow. The FPS uses Carbon Black (CB) dispersed in polydimethylsiloxane (PDMS) as a piezoresistive sensor layer, which is stencil printed on a structural PDMS layer. In this study, we analyze the strain transducer mechanisms on a vascular graft and show the linear and stable strain response of CB-PDMS composites from 0-50% strain. The material has a broader strain range than graft materials and a gauge factor of 5. In vitro testing of the FPS on a vascular graft phantom showed a robust, linear sensor output to pulsatile flows and pressures. The composite material shows excellent potential in biologic strain sensing applications where a flexible sensor with large maximum strain range is needed.

## 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 nanomechanical 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.

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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. The 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.

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# Tuesday Afternoon, October 22, 2019

**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  $h\nu = g\mu_B B \pm \sum_i m_i A_i$ , 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  $i^{\text{th}}$  nucleus, and  $A_i$  is the hyperfine interaction of the  $i^{\text{th}}$  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  $\mu\text{m}$ , 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  $\text{Er}_{\text{ad}}$  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  $\text{Er}_{\text{Ga}}$  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 experiments 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 outlining 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  $V_{\text{Si}}$  in 4H-SiC for Quantum Technologies using  $\text{Li}^+$  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 DeJarlid, 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 ( $V_{\text{Si}}$ ). 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  $V_{\text{Si}}$  within microcavities is necessary. Here we show implanted  $\text{Li}^+$  into Si-face, 4H-SiC homoepitaxy creates  $V_{\text{Si}}$  in desired locations. The epitaxial material had no measurable  $V_{\text{Si}}$  prior to  $\text{Li}^+$  implantation. The dose of 100 keV  $\text{Li}^+$  ranged from  $10^{12} - 10^{15} \text{ cm}^{-2}$  and was directed using a maskless focused ion beam technique with a positional accuracy of  $\sim 25 \text{ nm}$ . 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  $V_{\text{Si}}$  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 Greenspan, 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 ( $V_{\text{Si}}^-$ ) 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.  $V_{\text{Si}}^-$  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  $V_{\text{Si}}^-$  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  $V_{\text{Si}}^-$  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

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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 Puzetzy, L Liang, R Onocic, D Geohegan*, Oak Ridge National Laboratory

Two-dimensional (2D) materials are intrinsically heterogeneous, therefore controlling 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<sub>2</sub>, 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<sub>2-x</sub> but also create new antisite defects in monolayers of WS<sub>2</sub> 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°C in 1.5mTorr 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 ( $T_{\text{eff}}$ ) 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 ( $T_{\text{eff}}$ ) is observed. Therefore, the Coulomb resonance is not only thermally broadened by  $T_{\text{eff}}$  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  $T_{\text{eff}}$ . 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<sup>2</sup> 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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# Tuesday Evening Poster Sessions, October 22, 2019

## **MEMS and NEMS Group**

### **Room Union Station AB - Session MN-TuP**

#### **MEMS and NEMS Poster Session**

**MN-TuP-1 Multimodal & Multifunctional Soft Sensors for Electronic Textiles**, *Ashish Kapoor, T Ghosh, A Bozkurt*, North Carolina State University

Soft polymer-based sensors as an integral part of textile structures have attracted considerable scientific and commercial interest recently because of their potential use in healthcare, security systems, and other areas. While electronic sensing functionalities can be incorporated into textiles at one or more of the hierarchical levels of molecules, fibers, yarns, or fabrics, arguably a more practical and inconspicuous means to introduce the desired electrical characteristics is at the fiber level, using processes that are compatible to textiles. In this research, a prototype multimodal and multifunctional sensor array formed within a woven fabric structure using bicomponent fibers with ordered insulating and conducting segments is reported. The conducting segments are extruded from a percolating conducting composite made by dispersing carbon fillers in an elastomer. The multifunctional characteristics of the sensors are successfully demonstrated by measuring tactile, tensile, and shear deformations, as well as wetness and biopotential (heart rate). While the unobtrusive integration of sensing capabilities offer possibilities to preserve all desirable textile qualities, this approach demonstrates the potential for scalable and facile manufacturability of practical e-textile products. The capability of these fiber-based sensors is further being explored for objective monitoring of the inner socket environment (i.e. pressure, temperature, and humidity) and residual muscle activity during daily prosthesis use in lower limb amputees.

## 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 $\alpha$ - $\text{In}_2\text{Se}_3$ for Non-Volatile Memory Applications, *M Si, Peide Ye*, Purdue University

$\alpha$ - $\text{In}_2\text{Se}_3$  is a novel two-dimensional (2D) ferroelectric semiconductor. It has a bandgap of  $\sim 1.39$  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  $862 \mu\text{A}/\mu\text{m}$ , low supply voltage with scaled gate insulator and the potential to exceed the existing Fe-FETs for non-volatile memory applications.

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#### 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

$\text{NaSn}_2\text{As}_2$  has recently been synthesized and was found to be an exfoliable 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 David*, 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  $(\text{CH}_3(\text{CH}_2)_3\text{NH}_3)_2(\text{CH}_3\text{-NH}_3)_{n-1}\text{Pb}_n\text{I}_{3n+1}$  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  $\text{MoS}_2$  due to the much more deformable  $[\text{PbI}_6]^{4-}$  octahedral 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. For 2D 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  $[\text{PbI}_6]^{4-}$  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.

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#### 9:40am 2D+EM+MI+MN+NS+QS-WeM-6 Collective Electronic States of Epitaxial Monolayer 1T-NbSe<sub>2</sub>, *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<sub>2</sub> doesn't exist in nature, here we show that single layer 1T NbSe<sub>2</sub> 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<sub>2</sub> is also a Mott insulator, similar to that of bulk 1T TaS<sub>2</sub>. 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<sub>2</sub> will be discussed at the meeting.

#### 11:00am 2D+EM+MI+MN+NS+QS-WeM-10 Magnetic Interfaces of MnSe<sub>2</sub> 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 CrI<sub>3</sub> and Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub>. A different material, MnSe<sub>2</sub>, 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

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samples they report an interface of the MnSe<sub>2</sub> monolayer with bulk  $\alpha$ -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/functionality, 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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## Electronic Materials and Photonics Division

### Room A214 - Session EM+2D+AS+MI+MN+NS+TF-WeM

#### Nanostructures and Nanocharacterization of Electronic and Photonic Devices

**Moderators:** Sang M. Han, University of New Mexico, Jason Kawasaki, University of Wisconsin - Madison

8:00am **EM+2D+AS+MI+MN+NS+TF-WeM-1 Photonic Thermal Conduction in Semiconductor Nanowires**, *E Tervo*, *M Gustafson*, *Z Zhang*, *B Cola*, *Michael A. Filler*, Georgia Institute of Technology

We present a practical material system—chains of infrared plasmonic resonators situated along the length of semiconductor nanowires—where near-field electromagnetic coupling between neighboring resonators enables photonic thermal transport comparable to the electronic and phononic contributions. We model the thermal conductivity of Si and InAs nanowires as a function of nanowire diameter, resonator length, aspect ratio, and separation distance by combining discrete dipolar approximation calculations, to determine the relevant dispersion relations, with thermal kinetic theory. We show that photonic thermal conductivities exceeding  $1 \text{ W m}^{-1} \text{ K}^{-1}$  are possible for 10 nm diameter Si and InAs nanowires containing repeated resonators at 500 K, more than an order of magnitude higher than existing materials systems and on par with that possible with phonons and electrons. These results highlight the potential for photons in properly engineered solids to carry significant quantities of heat and suggest new ways to dynamic control thermal conductivity.

8:20am **EM+2D+AS+MI+MN+NS+TF-WeM-2 Electric Field-Induced Defect Migration and Dielectric Breakdown in ZnO Nanowires**, *Hantian Gao*, *M Haseman*, Department of Physics, The Ohio State University; *H von Wenckstern*, *M Grundmann*, Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik; *L Brillson*, The Ohio State University

Nanowires of the II-VI compound semiconductor ZnO have generated considerable interest for next generation opto- and microelectronics . Central to nanowire electronics is understanding and controlling native point defects, which can move<sup>1</sup> and lead to dielectric breakdown under applied electric fields. We used nanoscale lateral and depth-resolved cathodoluminescence spectroscopy (DRCLS) with hyperspectral imaging (HSI) in a scanning electron microscope (SEM) to observe defect migration and redistribution directly under applied electric fields and after dielectric breakdown. HSI maps represent lateral intensity distributions of specific features acquired pixel by pixel across SEM-scanned areas and normalized to near band edge (NBE) emissions. A pulsed layer deposited (PLD) ZnO microwire (3  $\mu\text{m}$  diameter) exhibited homogeneous distributions of common luminescence features at 2.0 eV ( $V_{\text{Zn}}$  cluster) and 2.35 eV ( $\text{Cu}_{\text{Zn}}$ ) as well as 2.7 and 2.9 eV ( $V_{\text{Zn}}$ ) peaks near the wire surface. With increasing electrical bias up to  $3 \times 10^5 \text{ V/cm}$  between two Pt contacts, these defects systematically redistribute, even at room temperature, moving toward and under one of the contacts, draining the “bulk” nanowire, especially its near-surface region. Since ionized  $V_{\text{Zn}}$ -related and  $\text{Cu}_{\text{Zn}}$  antisite defects are acceptors, their removal reduces the compensation of electron density in the typically n-type ZnO and thus its resistivity.

Besides HSI lateral maps, DRCLS vs. incident beam energy yields depth profiles radially of defects at specific locations along the nanowire. These exhibit high near-surface and wire core densities that biasing reduces. Current voltage measurements with increasing field gradients show a gradual resistivity decrease until an abrupt dielectric breakdown of the microwire at 300 kV/cm (150 V/5  $\mu\text{m}$ ). The acceptor removal between the contacts and their accumulation under one of the contacts can both contribute to this breakdown due to the decrease in resistivity and higher current conduction between the contacts and possible defect-assisted tunneling<sup>2</sup> across the increased defect density under the contact, respectively. These electric field-induced defect movements may be of more general significance in understanding dielectric breakdown mechanism not only in ZnO nanostructures but also bulk semiconductors in general.

HG, MH, and LJB gratefully acknowledge support from AFOSR Grant No. FA9550-18-1-0066 (A. Sayir). HVW and MG acknowledge Deutsche Forschungsgemeinschaft (Gr 1011/26- 1).

1. G. M. Foster, *et al.*, *Appl. Phys. Lett.* **111**, 101604 (2017).

2. J.W.Cox, *et al.*, *Nano Lett.* **18**, 6974 (2018).

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8:40am **EM+2D+AS+MI+MN+NS+TF-WeM-3 Characterization of SiGe/Si Multilayer FIN Structures using X-Ray Diffraction Reciprocal Space Maps**, **Roopa Gowda**, M Korde, SUNY Polytechnic Institute; M Wormington, Jordan Valley Semiconductors Inc.; A Diebold, SUNY Polytechnic Institute

Nanowire and Nanosheet FET's are potential replacements for FinFET's, mainly beyond sub-10nm CMOS technology nodes, as gate-all-around (GAA) FET device architecture provides improved electrostatics in higher on current ( $I_{on}$ ) and better subthreshold swing. As GAA is one of the best promising device for logic applications for future technology nodes, there is an increased need of characterization technique for such multilayer  $Si_{1-x}Ge_x/Si$  complex structures. We studied  $Si_{1-x}Ge_x/Si/Si_{1-x}Ge_x/Si/Si_{1-x}Ge_x/Si$  multilayer FIN structures using X-Ray Diffraction Reciprocal Space Maps (RSM). RSM is one of the most popular technique to study epitaxial thin-films nanostructures due to straightforward analysis of the data. We found RSM simulations showing sensitivity of nanosheet fin structures dimensions such as pitch-walk (PW), Nanosheet thickness (NST), composition and shape. RSM's provide better means to interpret more complex diffraction measurements than real space constructions. RSMs of  $Si_{1-x}Ge_x/Si$  multilayer structure has been simulated using Bruker Jv-RADS v6.5.50/HRXRD software. 1D line profiles extracted from RSMs was also used for the analysis of nanostructures dimensions. We obtained multilayer structure dimensions from the published information. We studied the influence of nanostructure parameters PW, NST, Composition and shape on RSMs. Imperfect periodic structures impact the intensity modulation of the grating rods (GRs). We observed that satellite peaks intensity reduces and harmonics peaks intensity enhances as PW increases. Rate of intensity change in higher order peaks is much faster than the lower harmonic peaks. We observed that the spacing between adjacent interference fringes in RSMs is related to the thickness of the layers. The period of fringes is inversely proportional to the thickness of the layer, hence total FIN height can be determined. 1D line profiles along  $Q_x$  shows decreased angular width and increase in intensity of the layer peak and interference fringes as NST increases. Symmetric 004 longitudinal RSMs and their line profiles clearly show layer peak shift from substrate peak as composition increases due to increase of SiGe lattice spacing along the growth direction. Cross-shaped GR pattern in RSMs is observed which is due to trapezoidal surface grating caused by SWA. Line profiles indicate that fin shapes influence the modulation of the GRs as a function of  $Q_x$ . We demonstrate the characterization of complex  $Si_{1-x}Ge_x/Si$  multilayers using RSMs and their line profiles which are relevant for lateral nanowire and nanosheet FETs. Above findings from RSM simulations clearly indicate the influence of variations in structural dimensions.

9:00am **EM+2D+AS+MI+MN+NS+TF-WeM-4 Nanoscale Depth and Lithiation Dependence of  $V_2O_5$  Band Structure by Cathodoluminescence Spectroscopy**, **Mitchell Walker**, N Pronin, The Ohio State University; A Jarry, J Ballard, G Rubloff, University of Maryland, College Park; L Brillson, The Ohio State University

Vanadium pentoxide ( $V_2O_5$ ) has attracted considerable interest for its potential use as a cathode for solid state lithium ion batteries. While researchers have studied the  $V_2O_5$  lithiation charge/discharge cycle for over two decades, we are only now able to measure directly its electronic band structure from the surface to the thin film bulk and its changes with Li intercalation on a near-nanometer scale. We used depth-resolved cathodoluminescence spectroscopy (DRCLS) to monitor the changes in electronic structure from the free surface to the thin film bulk several hundred nm below. DRCLS measures optical transitions at 1.8-2, 3.1-3.2, 3.6-3.7, 4.0-4.1, and 4.6-4.7 eV between multiple conduction bands to the pristine ( $\alpha$ )  $V_2O_5$  valence band maximum in excellent agreement with  $V_{3d}t_{2g}$  conduction band densities of states (DOS) predicted by density functional theory (DFT).<sup>1</sup> Triplet conduction band states at 1.8, 1.9, and 2 eV correspond to predicted  $V_{3d}t_{2g}-O_{2p_x/2p_y}$  hybridized states resulting from strong deviations of the unit cell  $VO_6$  octahedra from cubic coordination correspond to optical absorption edges along the 3 crystallographic axes. With excitation depth increasing from  $< 10$  to 125 nm calibrated by Monte Carlo simulations, the relative amplitudes and energies of these states change, signifying gradual changes in octahedral distortion. The band structure changes significantly with Li intercalation into  $Li_xV_2O_5$  for  $x = 0, 1,$  and 2. Lithiation gradually removes the hybridized band and introduces a 2.4-2.7 eV  $V_{3d}t_{2g}$  band extending 50 nm ( $x=1$ ) or 25 nm ( $x=2$ ) into the surface. Higher (4.0 and 4.4 eV) features possibly related to a secondary phase dominate the spectra deep inside all  $V_2O_5$  films near the battery electrode. Delithiation reintroduces the 1.8-2 eV split-off band although significantly narrowed by octahedral distortions. Overall, DRCLS shows that the lithiation cycle alters the  $V_2O_5$  band structure on a scale of 10-100's of

nm with lithiation. The direct measure of  $V_2O_5$ 's electronic band structure as a function of lithiation level provided by DRCLS can help guide future battery engineering work as more efficient lithium ion batteries are developed. In particular, these unique electrode measurements may reveal in what ways lithiation changes  $V_2O_5$  irreversibly, as well as reveal methods to extend solid state battery life. MW and LJB acknowledge support from NSF grant DMR-18-00130. AJ and GR acknowledge Nanostructures for Electrical Energy Storage (NEES), a Department of Energy Office of Science Frontier Research Center.

1. V. Eyert and K.-H. Höck, "Electronic structure of  $V_2O_5$ : Role of octahedral deformation," Phys. Rev. B 57, 12727 (1998).

9:20am **EM+2D+AS+MI+MN+NS+TF-WeM-5 Electron Microscopy of Quantum Materials: From Learning Physics to Atomic Manipulation**, **Sergei Kalinin**, Oak Ridge National Laboratory

**INVITED**

Atomically-resolved imaging of materials has become the mainstay of modern materials science, as enabled by advent of aberration corrected scanning transmission electron microscopy (STEM). In this talk, I will present the new opportunities enabled by physics-informed big data and machine learning technologies to extract physical information from static and dynamic STEM images. The deep learning models trained on theoretically simulated images or labeled library data demonstrate extremely high efficiency in extracting atomic coordinates and trajectories, converting massive volumes of statistical and dynamic data into structural descriptors. I further present a method to take advantage of atomic-scale observations of chemical and structural fluctuations and use them to build a generative model (including near-neighbour interactions) that can be used to predict the phase diagram of the system in a finite temperature and composition space. Similar approach is applied to probe the kinetics of solid-state reactions on a single defect level and defect formation in solids via atomic-scale observations. Finally, synergy of deep learning image analytics and real-time feedback further allows harnessing beam-induced atomic and bond dynamics to enable direct atom-by-atom fabrication. Examples of direct atomic motion over mesoscopic distances, engineered doping at selected lattice site, and assembly of multiatomic structures will be demonstrated. These advances position STEM towards transition from purely imaging tool for atomic-scale laboratory of electronic, phonon, and quantum phenomena in atomically-engineered structures.

11:00am **EM+2D+AS+MI+MN+NS+TF-WeM-10 Hot Electron Emission from Waveguide Integrated Graphene**, **Ragib Ahsan**, F Rezaeifar, H Chae, R Kapadia, University of Southern California

From free electron laser sources to electronic structure measurements, electron emission devices play an important role in a wide range of areas. Photoemission is one of the basic processes exploited in modern electron emission devices. However, higher-order processes like multiphoton absorption or optical field induced emission are necessary for efficient photoemission from high workfunction metallic emitters. Our work demonstrates a graphene emitter integrated on a waveguide that can evanescently couple with the photons delivered from a CW laser (405 nm) and registers photoemission at a peak power that is orders of magnitude lower than previously published results based on multiphoton and optical field induced emission processes. Coupling FDTD analysis of the waveguide to a rigorous quantum mechanical study of the scattering mechanisms and the tunneling processes in graphene, we have been able to model the emission current from the graphene emitter with good agreement to the experimental data. Our investigation reveals that the photoexcited electrons can go through three mutually competitive processes: (i) electron-electron scattering (ii) electron-phonon scattering and (iii) directly emission into the vacuum. Absorption of a photon causes a reduction in the tunnel barrier seen by the electron and the emission rate increases exponentially. Integration of graphene to the waveguide enables evanescent coupling between electrons and the photons causing almost 100% absorption of the photons. Our integrated photonics approach demonstrates an emission efficiency that is three orders of magnitude greater than free space excitation. These results suggest that integrating photonic elements with low dimensional materials such as 2D materials, nanoparticles, quantum dots, etc. can provide a new domain of efficient electron emission devices and integrated photonics.

11:20am **EM+2D+AS+MI+MN+NS+TF-WeM-11 Imaging Candidate Nanoelectronic Materials with Photoemission Electron Microscopy (PEEM)**, **Sujitra Pookpanratana**, S Robey, National Institute of Standards and Technology (NIST); T Ohta, Sandia National Laboratories

The drive to produce smaller and lower power electronic components for computing is pushing the semiconductor industry to consider novel

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nanoscale device structures, not based solely on crystalline silicon. Continued innovation and progress towards novel nanoelectronic materials and devices in turn requires metrologies sensitive to electronic properties at these length scales. Tip-based imaging techniques provide electronic contrast with sub-nanometer resolution, however it is a local, scanning-based technique. Photoemission (or photoelectron spectroscopy) is the dominant technique to provide detailed electronic band structure information- level energies, dispersion, polarization dependence, etc. – but typically requires materials with millimeter, or larger, length scales. Photoemission electron microscopy (PEEM) can be employed to allow access to this vital information, providing full-field imaging capabilities sensitive to a variety of electronic contrast mechanisms at 10's of nanometers length scales. Here, we will present our results on imaging the impact of molecular dopants on multilayer tungsten disulfide (WS<sub>2</sub>) employing the PEEM at the Center for Integrated Nanotechnologies within Sandia National Laboratories. We will also discuss the commissioning of a recently installed PEEM to perform complementary measurements at NIST-Gaithersburg.

Technological commercialization of transition metal dichalcogenides (TMDs) in nanoelectronics devices requires control of their electronic properties, such as charge carrier type and density, for specific device functionality. Conventional techniques for doping are problematic for atomically thin 2D materials. The sensitivity of mono- to few-layer (TMDs) to their local environment and interfaces can be employed *via* surface doping of molecules on TMDs to provide a promising route toward controllable doping. Investigations of surface doping for one to few layer WS<sub>2</sub> were performed using mechanically exfoliated WS<sub>2</sub> on a SiO<sub>2</sub>/Si substrate that was then exposed to tris(4-bromophenyl)ammonium hexachloroantimonate, a p-dopant molecule. PEEM was performed before and after p-dopant exposure. After doping, we find that the contrast of the surface WS<sub>2</sub> physical features change and valence band edge shifts about 0.8 eV away from the Fermi energy, consistent with p-doping. We will discuss the effects of molecular doping in terms of homogeneity and surface features across multiple WS<sub>2</sub> flakes. Lastly, we will discuss commissioning of a new PEEM instrument installed at NIST in 2019, using results of graphene to demonstrate imaging capability and energy resolution of this instrument.

11:40am **EM+2D+AS+MI+MN+NS+TF-WeM-12 Comparison of Features for Au and Ir Adsorbed on the Ge (110) Surface**, *Shirley Chiang*, University of California, Davis; *R Xie, H Xing*, Donghua University, China; *T Rahman*, University of Central Florida; *C Fong*, University of California, Davis

Two ad-atoms of Au and Ir adsorbed, respectively, on the Ge(110) surface are studied by a first-principles algorithm based on density functional theory. The surface is modeled by a slab consisting of 108 Ge atoms with a 10 Å vacuum region. Hydrogen atoms are used to saturate the dangling orbitals at the other side of the vacuum region. Two cases of Au adsorption and one case of Ir are reported. The case of Ir has a large binding energy because of its small atomic size compared with the Ge atom, and the partially filled d-states. The total energy for each case is given, as are the energies for removing one ad-atom at a time and also both ad-atoms. The binding energy of each case is obtained by simply taking the energy difference between these configurations; this method is more realistic because the experimental data measured by LEEM and STM indicate that the collective motions of the ad-atoms do not allow the surface to relax to its equilibrium state.[1] For a large separation in the case of two Au atoms, there is a smaller binding energy than for one ad-atom. This can relate to the fact that the collective motions seen experimentally do not happen at a full monolayer coverage of ad-atoms.[1] Additional comparisons will be made to an atomic model for Ir/Ge(111) from STM measurements.[2]

[1] B. H. Stenger et al., *Ultramicroscopy*, 183, 72 (2017).

[2] M. van Zijl et al., *Surf. Sci.* 666, 90, (2017).

Support from NSF DMR-1710748 (SC, CYF); NSF DMR-1710306 (TSR); National Natural Science Foundation of China Grants 61376102, 11174048 and computational support from Shanghai Supercomputer Center (RKX, HZX).

12:00pm **EM+2D+AS+MI+MN+NS+TF-WeM-13 Reference Materials for Localization Microscopy**, *C Copeland, R Dixon, L Elliott, B Ilic*, National Institute for Science and Technology (NIST); *D Kozak, K Liao*, FDA, National Institute for Science and Technology (NIST); *J Liddle*, NIST Center for Nanoscale Science and Technology; *A Madison*, National Institute for Science and Technology (NIST); *J Myung*, FDA; *A Pintar, Samuel Stavis*, National Institute for Science and Technology (NIST)

As the diffraction limit fades away into the history of optical microscopy, new challenges are emerging in super-resolution measurements of diverse systems ranging from catalysts to therapeutics. In particular, due to common limitations of reference materials and microscope calibrations, many localization measurements are precise but not accurate. This can result in gross overconfidence in measurement results with statistical uncertainties that are apparently impressive but potentially meaningless, due to the unknown presence of systematic errors that are orders of magnitude larger. To solve this fundamental problem in measurement science, we are optimizing and applying nanofabrication processes to develop reference materials for localization microscopy, and demonstrating their use in quantitative methods of microscope calibration.

Our program consists of two complementary approaches. In the first, involving applied metrology, we are developing reference materials such as aperture arrays that can serve as standalone artifacts for widespread deployment. This approach will require the application of critical-dimension metrology to establish the traceability of master artifacts, and their use to calibrate a super-resolution microscope for high-throughput characterization of economical batches of reference materials. In the second approach, involving fundamental research, we are demonstrating the application of reference materials and calibration methods in our own experimental measurements. Most interestingly, achieving vertical integration of our two approaches and the unique capabilities that result, we are building reference materials into measurement devices for in situ calibration of localization measurements for nanoparticle characterization.

## 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.

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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 Standards 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

[2] S. J. Whiteley *et al.*, Nature Phys. **15**, 490 (2019)

**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 nanoindentations, 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. Here I will



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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+MN+NS-WeA

#### 2D Device Physics and Applications

Moderator: Jyoti Katoch, Carnegie Mellon University

2:20pm **2D+EM+MN+NS-WeA-1 Monolayer Electronics and Optoelectronics - Advances, Opportunities and Challenges, Ali Javey, University of California at Berkeley** **INVITED**

Two-dimensional semiconductors exhibit excellent device characteristics, as well as novel optical, electrical, and optoelectronic characteristics. In this talk, I will present our recent advancements in surface passivation, contact engineering, surface charge transfer doping, and heterostructure devices of layered chalcogenides. We have developed a passivation technique that allows for observation of near-unity photoluminescence quantum yield in monolayer semiconductors. I will discuss the mechanism by which non-radiative recombination can be fully removed in monolayers. The work presents the first demonstration of an optoelectronically perfect monolayer, and highlights one of their unique properties. Finally, I will discuss an AC carrier injection mechanism to enable bright light emitting devices using monolayers, overcoming the problem of Schottky contacts.

3:00pm **2D+EM+MN+NS-WeA-3 Investigation on Graphene Band-gap Engineering for Graphene Transistors Applications, Benfdila Arezki, University M. Mammeri Tizi-Ouzou, Algeria**

Graphene transistors are considered to be the successor's basic element for the next generation of advanced integrated circuits. However, graphene material suffers from the absence of bandgap to behave as semiconductor. The present paper deals with the investigation on the bandgap engineering approach aiming an increase of the switching characteristics of the graphene transistors.

The main obstacle for graphene transistor is the material zero bandgap that worsens the switching characteristics of the GFETs. Several techniques have been proposed to open a bandgap in graphene, among these engineering techniques, we can cite the Substrate induced bandgap, Bandgap engineering using h-BN/Ni (111). It is known that in theory a maximum of 0.50 to 0.53 eV can be obtained. Such bandgaps are observed on Graphene Bi-Layer (GBL) sheets grown on silicon carbide (SiC).

Other methods are the substitutional doping (SD), Nitrogen doping (NB). In any case graphene engineering should be considered in chemistry and physics view points. A high selective hydrogenation of graphene grown by lithography under the form of nanoruban showed a very interesting result of 0.7 eV. This process is part of selective chemical graphene functionalization techniques (SCGF).

In this paper we will deal with the graphene nanoruban and the opening of a bandgap capable of inducing an appreciable switching current ratio of at least  $I_{ON}/I_{OFF} > 10^6$ .

The Graphene Nano Ribbon (GNR) structure used in the form of GNR/FET for logic circuits and RF devices combines the high field, high mobility and the possibility of opening a bandgap. The higher carrier mobility of graphene is the basis of all electrical characteristics of graphene transistors.

In this paper we have used a semi-classical device model including the band to band tunneling that is described in Ref<sup>6</sup> to emphasize on the bandgap engineering. Device performances are studied based on the current-voltage characteristics with respective bandgap width variations.  $I_{OFF}$  current estimated and the performance ratio deduced.

3:20pm **2D+EM+MN+NS-WeA-4 Fully Inkjet Printed, High Photo-responsive, 2D WSe<sub>2</sub>-Graphene Based Flexible Photodetector, R Hossain, A Kaul, Avra Bandyopadhyay, University of North Texas**

Tungsten di-selenide (WSe<sub>2</sub>), a classic representative of two dimensional (2D) layered materials has recently drawn much attention due to its unique optoelectronic properties, offering a potential platform to construct hetero-structure photodetector (PD) for ultrafast optoelectronic devices on low-cost, flexible substrates [1,2]. As WSe<sub>2</sub> exhibits a weak van der Waals interlayer bonding, one of the approaches to obtain 2D WSe<sub>2</sub> is through top-down liquid phase exfoliation (LPE), where the bulk crystal is dispersed in a solvent through appropriate sonication and centrifugation conditions [1]. In this work, we report on the synthesis of WSe<sub>2</sub> via LPE and the first-ever assembly of an all inkjet printed WSe<sub>2</sub>-graphene hetero-structure PD on flexible polyimide film, where the WSe<sub>2</sub> acted as a photo-active semiconductor and graphene was the carrier collector. The inkjet printed PD was photo-responsive to broadband incoming radiation in the visible regime, and exhibited a high photoresponsivity  $R \sim 0.70$  A/W, and

detectivity  $D \sim 3 \times 10^{10}$  Jones. The strain-dependent measurements were conducted with bending for different curvatures, indicating the feasibility of such devices for large format arrays printed on flexible substrates. The capacitance-frequency ( $C-f$ ) measurements were performed to investigate the trap states. In conclusion, this unique all inkjet printed 2D hetero-junction photodetector formed on flexible and conformable substrate was successfully shown to be highly photo-responsive to a wide range of light intensities and strain levels, making it a promising prospect for scalable flexible electronic and optoelectronic devices and circuitry.

#### References:

[1] Kelly, A. G., Hallam, T., Backes, C., Harvey, A., Esmaeily, A. S., Godwin, I., ... & Kinge, S. (2017). All-printed thin-film transistors from networks of liquid-exfoliated nanosheets. *Science*, 356(6333), 69-73.

[2] Pradhan, N. R., Ludwig, J., Lu, Z., Rhodes, D., Bishop, M. M., Thirunavukkuarasu, K., ... & Balicas, L. (2015). High photoresponsivity and short photoresponse times in few-layered WSe<sub>2</sub> transistors. *ACS applied materials & interfaces*, 7(22), 12080-12088.

4:20pm **2D+EM+MN+NS-WeA-7 Chemical Vapor Sensing with Transition Metal Dichalcogenides via Photoluminescence Modulation, Aubrey T. Hanbicki, P Campbell, S Sivaram, U.S. Naval Research Laboratory; A Kusterbeck, Nova Research, Inc.; V Nguyen, A McGill, K McCreary, B Jonker, E Cobas, K Perkins, U.S. Naval Research Laboratory; A Friedman, Laboratory for Physical Sciences**

Two-dimensional transition metal dichalcogenides (TMDs) such as MoS<sub>2</sub> and MoSe<sub>2</sub> are promising materials for chemical vapor sensing applications. Their potential includes straightforward fabrication, readily available materials, and good selectivity, sensitivity, and speed of response. We previously showed [1] that monolayer TMDs are sensitive to and selective for vapors of strong electron donors and/or strong electron acceptors in concentrations as low as 1 part per million (ppm). Another attractive aspect is that TMDs have been shown to detect chemical vapors and gases in several ways, for instance via changes in electrical conductance or photoluminescence (PL) [2]. Sensors commonly have been fabricated based on the chemiresistive device properties, but here we will discuss our recent studies implementing TMD sensors using the PL as the core element of the sensor. We show that the PL intensity of monolayer CVD-grown WS<sub>2</sub> can rapidly (<< 1sec) detect triethylamine (TEA), a decomposition byproduct of the VX series of nerve agents, in concentrations <<1 ppm. The optical response is similar to the electrical response of other TMDs previously shown [1]. We shall discuss the mechanisms determining the size and shape of the optical responses. We envision suites of different TMDs using both optical and conductance sensing to rapidly and selectively detect chemical agents.

This research was performed while S.V.S held a National Research Council fellowship at NRL. This work was supported by core programs at NRL.

#### References

[1] A.L. Friedman et al., *Sci. Reports* 7, 3836 (2017)

[2] P.M. Campbell et al., *Appl. Phys. Lett.* 113, 163106 (2018)

4:40pm **2D+EM+MN+NS-WeA-8 Effective and Robust Graphene Immunological Sensors Functionalized through Non-covalent Ninding of Antibody-Conjugated Tripodal Compound, A Hugo, CEA-LETI, France; C Sun, Northwestern University; M Kumar, CEA-LETI, France; R Othmen, J Renard, V Bouchiat, CNRS-Institut Néel, France; J Mann, Northwestern University; J Parpia, H Craighead, Cornell University; P Mailley, CEA-LETI, France; W Dichtel, Northwestern University; Thomas ALAVA, CEA-LETI, France**

Electrical detection is a very robust technique to transduce the adsorption of charged protein to a biological selective layer (i.e. biosensing). Electrolyte gated field effect transistors (EGFET) integrating graphene monolayers as the transducing element have shown outstanding electrical sensitivity in liquid compared to silicon and diamond based EGFET. In order to build graphene EGFET as effective biosensing unit it is important to attach at its surface a functional layers of biological molecules that will carry the task of enforcing specific detection of compound. Protein are widely used as specific bioreceptor for sensor biological functionalization yet it has been shown that protein lose their function when simply adsorbed on graphene. Covalent binding being out of the way for 2D dimensional crystals such as graphene (for the inherent deterioration of mechanical and electrical properties) we have shown that custom made tripodal compound attaching the graphene basal plane through Pi-stacking of aromatic moieties could be used to attach specific biomolecules to graphene while maintaining their biological function hence their specificity.

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In this report we present an optimized fabrication process for graphene EGFET that includes patterning and passivation of electrical contact. The devices reproducibly show state of the art electrical performances. We demonstrate that the process can be simply transferred to different host substrates to integrate graphene EGFET ubiquitously on Silicon, glass or printed circuit board with similar performances. Finally, we implemented biological functionalization of the sensors by attaching streptavidin to the sensor thanks to the non-covalent tripodal compound. We report consistent changes in the Dirac peak of graphene due to the adsorption of tripodal compound and streptavidin as well as the binding of biotin, specifically bound to streptavidin. We show the detection to be specific and reproducible.

5:00pm **2D+EM+MN+NS-WeA-9 Electronic Properties of Ultra-Thin Na<sub>3</sub>Bi: A Platform for a Topological Transistor, Mark Edmonds, Monash University, Australia**

**INVITED**

Na<sub>3</sub>Bi in bulk form represents a zero-bandgap topological Dirac semimetal (TDS), but when confined to few-layers is predicted to be a quantum spin Hall insulator with bulk bandgap of 300 meV.<sup>1</sup> Furthermore, application of an electric field to few-layer Na<sub>3</sub>Bi has been predicted to induce a topological phase transition from conventional to topological insulator.<sup>2</sup>

I will discuss our efforts to grow epitaxial few-layer Na<sub>3</sub>Bi via molecular beam epitaxy, and probe its electronic structure and response to an electric field using scanning probe microscopy/spectroscopy and angle-resolved photoelectron spectroscopy. We demonstrate that monolayer and bilayer Na<sub>3</sub>Bi are wide bandgap quantum spin Hall insulators ( $E_g > 300$  meV) that can be tuned with an electric field to semi-metallic, and at higher electric fields re-opened as a conventional insulator.<sup>3</sup> This is the first experimental demonstration of such an electric field tuned topological phase transition in any material. Finally, I will discuss our most recent efforts to perform transport measurements on few-layer Na<sub>3</sub>Bi at doping levels corresponding to bulk conduction and edge conduction, with and without an applied magnetic field.

## References

- [1] C. Niu et al., Phys. Rev. B (2017) 95, 075404
- [2] H. Pan et al., Scientific Reports (2015) 5, 14639
- [3] J. Collins et al., Nature 564, 390 (2018)

5:40pm **2D+EM+MN+NS-WeA-11 Transparent Conductive Oxides in Contact with 2-D Materials, Ravindra Mehta, A Bandyopadhyay, A Kaul, University of North Texas**

Combining two-dimensional materials with transparent conductive oxide can result in a fully transparent 2D electronics with outstanding device performance. It has been shown that monolayer MoS<sub>2</sub> in contact with AZO has 85% transmittance in the visible region, a low threshold voltage (0.69V) and a large switching ratio ( $4 \times 10^8$ ). Another study has shown that using 2D MoS<sub>2</sub> as an active channel, tin doped indium oxide as a backgated electrode and zinc doped indium oxide (IZO) as source-drain electrodes, 85% transmittance in the visible region can be obtained. The contact resistance between the IZO and MoS<sub>2</sub> was reduced after laser annealing which in turn enhances  $\mu_{\text{eff}}$  and  $I_{\text{on}}/I_{\text{off}}$ . Thus, it becomes essential to study the performance of different transparent conductive oxides in contact with various 2D materials in a transistor. Black phosphorus is an interesting 2D materials since it combines unique attributes of both transition metal dichalcogenides and graphene. CVD is a preferred method compared to other techniques such as mechanical exfoliation, liquid exfoliation, and PVD to synthesize 2D materials since the materials produced are of great quality as is a scalable technique. However, CVD of black phosphorus is challenging. Thus, CVD in addition to exfoliation will be used to develop 2D materials. In this work opto-electronics performance of various transparent conductive oxides in contact with different 2D materials is evaluated with an emphasis on black phosphorus.

6:00pm **2D+EM+MN+NS-WeA-12 Negative Fermi-level Pinning Effect Induced by Graphene Interlayer in Metal/Graphene/Semiconductor Junction, H Yoon, W Song, Ulsan National Institute of Science and Technology (UNIST), Republic of Korea; S Jung, SK Hynix, Republic of Korea; J Kim, Ulsan National Institute of Science and Technology (UNIST); K Mo, G Choi, H Jeong, J Lee, Kibog Park, Ulsan National Institute of Science and Technology (UNIST), Republic of Korea**

We report the direct observation revealing that the electric dipole layer originating from the off-centric distribution of interacting electrons at metal/graphene interface can induce the negative Fermi-level pinning effect in metal/graphene/semiconductor junction made on a semiconductor substrate containing regions with low interface-trap density. The graphene interlayer takes a role of diffusion barrier preventing the atomic intermixing at interface and preserving the low interface-trap density region. The change of electrostatic potential across the metal/graphene interface due to the interaction dipole layer and the doping of graphene is found to cause the negative Fermi-level pinning effect, supported by the Schottky barrier decreasing as metal work-function increasing. In case of metal/graphene/GaAs junction, the local small patches with very thin or no native oxide layer are considered to be responsible for the negative Fermi-level pinning. In the prevailing region with normal native oxides surrounding the small patches, the Fermi-level pinning appears to be strong. Meanwhile, the negative Fermi-level pinning is found to occur globally in metal/graphene/SiC junction where the SiC substrate is known to produce a low density of interface traps. This work provides an experimental method to form Schottky and Ohmic-like contacts simultaneously on a semiconductor substrate covered partially with graphene by using identical metal electrodes.

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## 2D Materials

### Room A216 - Session 2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA

#### Surface Chemistry, Functionalization, Bio, Energy and Sensor Applications

Moderator: Mark Edmonds, Monash University, Australia

2:20pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-1 Molecular Layers on Nanoporous Gold Electrodes, Elizabeth Landis**, College of the Holy Cross  
Nanoporous gold presents a surface with high conductivity and surface area, which makes it an interesting platform for surface chemistry. However, the nanoporous gold surface lacks the functionality necessary for many applications including sensing. We have investigated self-assembled thiol-based monolayers and the electroreduction of diazonium-based salts to form aryl molecular layers on nanoporous gold. We use infrared spectroscopy and cyclic voltammetry to show that the molecular layer ordering and density depends on the functionalization method, and the underlying nanoporous surface impacts molecular ordering and electron transfer properties.

2:40pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-2 Thermotropic Liquid Crystal (5CB) on Two-dimensional Materials, Paul Brown**, American Society for Engineering Education; *S Fischer, J Kofacz, C Spillmann, D Gunlycke*, U.S. Naval Research Laboratory

Current means of redirecting light often rely on either bulky mechanical gimbals or non-mechanical diffractive elements. The former often suffer from wear and are susceptible to failure, while the latter may have significant optical power confined within side lobes. One promising non-mechanical approach that can overcome present limitations in beam redirection incorporates liquid crystal (LC) for continuous, refractive steering. Nematogens, the molecules comprising the LC in a nematic phase, support inherent anisotropic optical and dielectric properties that result from local ordering of single molecules. Recent research suggests the possibility of including two-dimensional materials to act as both an alignment layer and electrode to LC. This offers the possibility of further reducing device dimensions and device response time. Yet little research has focused on the ground state properties of a nematogen interfacing with the two-dimensional substrate. In this talk, we present density functional theory results of the electronic properties of a well-known nematogen (5CB) interacting with graphene, boron nitride, and phosphorene. We also discuss the influence of an introduced single vacancy on the electronic properties of the composite system. We find that 5CB on phosphorene offers the strongest binding of the considered nanosheets. Moreover, we observe qualitatively different band alignments, and focus in particular on type I, which prohibits free carrier transfer between the substrate and nematic LC. Lastly, we discuss the impact of single vacancies on the performance of two-dimensional materials to operate as both an alignment layer and electrode for LC-based applications.

*This work has been supported by the Office of Naval Research, directly and through the U.S. Naval Research Laboratory.*

3:00pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-3 Is it Possible to Achieve Intra-molecular Resolution with Ambient AFM?, Vladimir Korolkov**, Oxford Instruments-Asylum Research; *S Chulkov, M Watkins*, University of Lincoln, UK; *P Beton*, The University of Nottingham, UK

Although achieving molecular resolution is now almost a routine across various SPM imaging modes, resolving the actual molecular structure at the atomic level has only been accomplished with NC-AFM in UHV often at low temperatures and with a functionalized probe. Of course, the ultimate goal in SPM is to resolve the chemical structure of a molecule identifying each atom.

In this work we are presenting an approach to achieve intra-molecular resolution on adsorbed molecules in the ambient at room temperatures with a standard AFM cantilever with unmodified tip. We have discovered that using a combination of higher eigenmodes and low oscillation amplitudes (~3-5Å) of a standard Si-cantilever routinely provides ultra-high resolution on adsorbed molecules on surfaces<sup>1,2</sup> and bulk polymers<sup>3</sup>.

With this approach we have been able to observe both intra-molecular features and inter-molecular contrast in thin films of coronene and melem molecules on the surface of hexagonal boron nitride (hBN). In case of coronene, all six benzene rings have been resolved as well as underlying atomic lattice of hBN. Unlike coronene, melem forms molecular assemblies with square symmetry stabilized with in-plane strong hydrogen bonds between amino groups. We have observed a strong inter-molecular

contrast where the hydrogen bonds are expected to be. Similar to coronene, the observed intra-molecular contrast was associated with three triazine rings. We have used Probe particle model<sup>4</sup> to simulate our experimental AFM images and found very good agreement between them. In fact, PPM allowed us a correct interpretation of melem square phase assembly.

Both systems were studied at room and elevated temperatures where we observed phase transitions leading to thermodynamically stable systems. The experimental results are in excellent agreement with density functional theory calculations.

We believe the proposed approach, yet still in its infancy, could potentially provide a pathway to unambiguous identification of molecules on surfaces in the ambient on standard AFM systems.

<sup>1</sup>Korolkov et al., Nat. Chem., 2017

<sup>2</sup>Korolkov et al., Nat. Comm., 2017

<sup>3</sup>Korolkov et al., Nat. Comm., 2019

<sup>4</sup>Hapala et al., Phys. Rev. B 90, 085421

3:20pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-4 Tailoring Surface Properties via Functionalized Hydrofluorinated Graphene Compounds, Jangyup Son**, University of Illinois at Urbana-Champaign; *N Buzov*, University of California at Santa Barbara; *S Chen*, University of Illinois at Urbana-Champaign; *D Sung*, Sejong University, Republic of Korea; *H Ryu*, Seoul National University, Republic of Korea; *J Kwon*, Yonsei University, Republic of Korea; *S Kim, J Xu*, University of Illinois at Urbana-Champaign; *S Hong*, Sejong University, Republic of Korea; *W King*, University of Illinois at Urbana-Champaign; *G Lee*, Seoul National University, Republic of Korea; *A van der Zande*, University of Illinois at Urbana-Champaign

Mixing compounds or alloys is an important process to tailor or enhance the intrinsic properties of materials such as chemical reactivity, mechanical strength, and electronic structure. In nanosystems, such as two-dimensional (2D) materials like graphene, transition metal dichalcogenides (TMDCs), and hexagonal boron nitride (hBN), where there is no distinction between the surface and the bulk, mixing of elements is also an important tool for tailoring the interaction of the material with its environment. A successful strategy for manipulating the chemical structures of 2D materials is the chemical functionalization of graphene with single elements such as H, O, N, and F. Yet, an even wider parameter space is possible by combining these functionalization species to produce ternary functionalized graphene compounds.

Here we present a new strategy for producing functionalized graphene compounds through the systematic control of the ratio between adatoms. We demonstrate tailored hydrofluorinated graphene (HFG) compounds via the sequential exposure of graphene to low-energy hydrogen plasma and xenon difluoride (XeF<sub>2</sub>) gas. We demonstrate reversible switching of the surface between completely hydrogenated graphene (HG) and fluorinated graphene (FG) as well as the intermediate ratio between two extremes. Moreover, we demonstrate pattern the surface functionalization on a single chip into chemically distinct materials (graphene, FG, HG, and HFG compounds).

Finally, with these patterned structures, we demonstrated tailoring of the surface and electronic properties of the 2D materials. First, the patterned structures enable direct comparisons of the relative surface properties such as wettability and surface friction. Additionally, the electrical properties of functionalized graphene compounds showed unusual recovery of electrical conductance during the partial transformation of FG to HFG, due to initial removal of existing F adatoms when exposed to hydrogen plasma. This study opens a new class of 2D compound materials and innovative chemical patterning that can lead to atomically thin 2D circuits consisting of chemically/electrically modulated regions.

4:00pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-6 Functionalization of MoS<sub>2</sub> with Halogens, G Copetti**, IF-UFRGS, Brazil; *E Nunes*, IQ-UFRGS, Brazil; *G Soares*, IF-UFRGS, Brazil; *Cláudio Radtke*, IQ-UFRGS, Brazil

Transition metal dichalcogenides (TMDs) with lamellar structures similar to that of graphite have received significant attention because some of them are semiconductors with sizable bandgaps and are naturally abundant. This offers opportunities for fundamental and technological research in a variety of fields including catalysis, energy storage, sensing, and electronic devices. In order to TMDs fulfill their potential, a precise control i) of surface functionalization and ii) of the number of stacked TMD monolayers are mandatory. Surface functionalization was shown to play a key role in

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tuning photoluminescence properties of MoS<sub>2</sub>, formation of controllable and low defect density dielectric/MoS<sub>2</sub> interfaces obtained by atomic layer deposition, and etching of MoS<sub>2</sub> layers. Halogenation is one of the most promising functionalization techniques of TMDs. MoS<sub>2</sub> etching with atomic layer control was already achieved by chlorine adsorption associated with Ar<sup>+</sup> sputtering. Moreover, doping techniques to tune the conductivity and photoemission properties of MoS<sub>2</sub> are essential. Previous works have already shown that incorporation of F-containing species in MoS<sub>2</sub> leads to doping, as well as other interesting properties such as tunable ferromagnetic ordering. In this work, we performed first principal calculations with the density functional theory (DFT) to gain insight into the effect of MoS<sub>2</sub> exposure to halogens. Results evidenced different reactivities while comparing F and Cl, as well as MoS<sub>2</sub> surfaces with variable amounts of defects. These results were explored experimentally. Bulk exfoliated MoS<sub>2</sub> as well as CVD-grown monolayer MoS<sub>2</sub> samples were used. Chlorination was achieved by irradiating the samples with UV light in Cl<sub>2</sub> flux. Prior to chlorination, sputtering of the MoS<sub>2</sub> with Ar ions is performed to induce S removal. X-ray Photoemission Spectroscopy measurements and Rutherford Backscattering Spectrometry showed that S vacancies play a fundamental role in the chlorination process, with vacancy concentration dictating the balance between etching of the MoS<sub>2</sub> layer and Cl incorporation. Fluorination was performed by exposing the samples to pulses of XeF<sub>2</sub>. Different degrees of fluorination are achieved by varying exposure time. S is removed and F is incorporated without any loss of Mo. Chemical displacement on the Mo 3d and S 2p XPS peaks was observed after both halogenations processes. These results can clarify the mechanisms of Cl and F incorporation. Finally, the halogenation techniques proposed can be simple and useful methods to adapt the MoS<sub>2</sub> properties for future applications.

4:20pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-7 Towards Higher Alcohol Synthesis from Syngas on 2D material-based catalysts: A First-Principles Study\***, *Tao Jiang, D Le, T Rahman*, University of Central Florida

Synthesis of higher alcohol from syngas has been of great interest owing to the limited petroleum resources and environmental concerns. Rational designing of cheap and efficient catalyst material for such synthesis is in great demand because of diminishing supply of the current state-of-the-art catalysts. Two dimensional (2D) materials are emerging with far-reaching potential for technical and industrial applications thanks to their unique properties, recent developments and improvement of production technologies. In this talk, we will discuss our recent work, based on first principles calculations, towards the unitization of 2D materials as catalysts for higher alcohol synthesis. In particular, defect laden hexagonal boron nitride (*dh*-BN) with N vacancies is excellent catalyst for hydrogenation of CO<sub>2</sub> towards ethanol formation, in the reaction pathway of which the crucial step for forming C<sub>2</sub> bond, i.e. reaction of adsorbed species CH<sub>3</sub>\* and CO\* to form CH<sub>3</sub>CO\*, is exothermic with reasonably low activation barrier (0.68 eV). On the other hand, we also find single layer of MoS<sub>2</sub> functionalized with small Au nanoparticle to catalyze CO hydrogenation reaction towards ethanol formation. Among all the elementary reactions, the important steps are the reaction of an adsorbed CH<sub>3</sub>\* and a CO\* molecule and the hydrogenation of acetyl to acetaldehyde (both are exothermic with activation barriers of 0.69 and 0.47 eV, respectively) to form C<sub>2</sub> species.[1] The results suggest that 2D materials are suitable candidates for higher alcohol synthesis. Full reaction pathways will be discussed together with results of Kinetic Monte Carlo simulations to shed light on the selectivity of the catalysts. Contact will be made with experimental data that validate our theoretical predictions.

[1] K. Almeida, K. Chagoya, A. Felix, T. Jiang et al, "Towards Higher Alcohol Formation using a single-layer MoS<sub>2</sub> activated Au on Silica: Methanol Carbonylation to Acetaldehyde", submitted

\*Work supported in part by DOE Grant DE-FG02-07ER15842

4:40pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-8 Proton Conductivity Properties of Electrospun Chitosan Nanofibers**, *Woo-Kyung Lee, J Pietron, D Kidwell, J Robinson, C McGann, S Mulvaney*, U.S. Naval Research Laboratory

A major challenge of the 21<sup>st</sup> century will be to establish meaningful two-way communication between biology and electronics. The study of protonics, devices that mimic electronics but pass protons instead of electrons, seeks to bridge this gap. Protonic conductive materials (PCMs) are essential elements of these devices and we have demonstrated significant improvement in conductivity for chitosan PCMs when deposited as electrospun nanofibers. The observed improvements stem from both enhanced molecular alignment and from chemical doping due to the

electrospinning carrier fluid, trifluoroacetic acid (TFA). We deposited electrospun chitosan nanofibers over palladium protodes and then used the helium ion microscope to isolate single nanofibers for detailed study. We observed that single chitosan nanofibers are strongly doped by TFA with x-ray photoelectron spectroscopy demonstrating extensively protonated nitrogen functionality. With the isolated, single chitosan nanofibers we observed that water uptake, fiber/electrode contact area, and doping concentration are critical parameters of protonic device performance and lead to increased conductivity (*i.e.* low resistivity). The average resistivity of single chitosan nanofibers is  $6.2 \times 10^4 \Omega\text{-cm}$ , approximately two orders of magnitude lower than the resistivity of cast chitosan PCMs (cast from acetic acid solutions not TFA). We have observed excellent agreement between theoretical models and experiment results that explore each of the contributions to the improved conductivity. In addition, the fabrication and measurement of ionic field-effect transistor of single chitosan fiber using conductive atomic force microscope will be discussed.

5:00pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-9 Sensor for Breath and Skin Diagnostics**, *Pelagia I Gouma*, The Ohio State University

Resistive gas sensors have received a bad reputation of being largely non-selective.

Our work has produced a crystallo-chemical model for selective gas sensing by polymorphic

metal oxides. The reaction-based and ferro-electric poling sensing mechanisms are discussed

in detail. Novel processing methods to produce the respective nano sensors are presented along

with the device fabrication for the non-invasive diagnosis of gaseous biomarkers in human

and animal breath or skin. This sensor technology is expected to revolutionize medical diagnostics.

5:20pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-10 Symmetry Controlled Adsorption of Diiodobenzene on MoS<sub>2</sub>**, *Zahra Hooshmand*, University of Central Florida; *P Evans, P Dowben*, University of Nebraska - Lincoln; *T Rahman*, University of Central Florida

In a joint experimental and theoretical study, we have uncovered evidence of the importance of symmetry in the adsorption of the isomers of diiodobenzene on MoS<sub>2</sub>(0001). The intensity ratio of iodine to molybdenum measured, as a function of exposure for different isomers of the diiodobenzene, show that while for ortho (1,2-) and para (1,4-) diiodobenzene the rate of adsorption at 100 K is very low, that for meta (1,3-) diiodobenzene is considerably more facile. We have applied dispersion corrected density functional theory-based calculations to understand the subtleties in the electronic structure and geometry of adsorption of these diiodobenzene isomers on MoS<sub>2</sub>(0001). All three isomers are found to weakly chemisorb with the same binding strength as well as adopt similar configurations. The calculated electron affinity of the three molecules also do not show a specific trend that would verify experimental data. However, analysis of the frontier orbitals indicate that those of 1,3-diiodobenzene are strongly affected by interactions with MoS<sub>2</sub>, while that of the other two isomers remain unchanged. Our results show that symmetry is the identifying factor in these adsorption characteristics. The results of frontier orbitals analysis confirm that for adsorption of (1,2-) and (1,4-) diiodobenzene a reduction in the symmetry of the adsorbent is needed. To further validate our conclusions, we compare the above results with that of the adsorption of the diiodobenzene isomers on defect-laden MoS<sub>2</sub>(0001).

\* Work support in part by DOE grant DE-FG02-07ER15842

5:40pm **2D+AS+BI+HC+MN+NS+PS+SS+TL-ThA-11 Mechanistic Understanding of the CO Hydrogenation Reaction on Defect Engineered 2D-TaS<sub>2</sub> and 2D-MoS<sub>2</sub> Catalysts**, *Mihai Vaida*, University of Central Florida

Due to global energy demands, investigation of catalytic reaction mechanisms on novel catalytic materials that can lead to efficient production of storable fuels from sustainable inputs is of central importance. In this contribution the adsorption of CO and H<sub>2</sub> molecules, as well as the CO hydrogenation reaction are investigated on defect engineered two dimensional (2D) TaS<sub>2</sub> and MoS<sub>2</sub>. Crystalline 2D-TaS<sub>2</sub> and 2D-MoS<sub>2</sub> with surface area of 1 cm<sup>2</sup> are synthesized via a multistep process based physical vapor deposition on Cu(111). The surface composition, morphology, and electronic structure are investigated via Auger electron spectroscopy, low energy electron diffraction, scanning tunneling

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microscopy, scanning tunneling spectroscopy, and photoemission spectroscopy. The interaction of the molecules with the surface and the catalytic reaction mechanisms are investigated via temperature programmed desorption/reaction. No catalytic reactions have been observed on crystalline 2D materials. However, an enhanced catalytic activity is observed after the generation of sulfur vacancies via Ar sputtering. The CO hydrogenation on TaS<sub>2</sub> occurs on low coordinated Ta atoms through the formation of formyl radical (HCO) and formaldehyde (HCOH). On 2D-MoS<sub>2</sub>, the CO hydrogenation also occurs on low coordinated Mo atoms. However, in this case the formyl radical splits to form methyldyne radical (CH), which subsequently react with other CH radical to produce acetylene (C<sub>2</sub>H<sub>2</sub>).

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