MEMS and NEMS Technical Group
Room 302 - Session MN+AS+NS+QS+SE-MoM

Dynamics and Engineering of MEMS/NEMS

Moderators: Jürgen Brugger, EPFL, Switzerland, **Eva Weig**, University of Munich, Germany

9:00am **MN+AS+NS+QS+SE-MoM-3 MEMS-Based Surface Nanoengineering Using Thermal AFM Probes: 30 Years and Counting**, ***Jürgen Brugger,*** École Polytechnique Fédérale de Lausanne, Switzerland **INVITED**

Soon after the first publication in 1985 of the atomic force microscope (AFM) attempts were made to extend AFM-based surface probing from microscopy to lithography [reviewed in 1]. The potential applications in writing and reading for data storagein the early years served as technology driver and showed remarkable performances [2]. One of the variants of AFM-based writing (and reading) operates a heated nano-tip to perform thermally induced phase changes of materials. The three-fold combination of nano-scale heat localization (30 nm scale), high temperature (~ 500 °C)and particularly fast heating/cooling cycles (10E-6 s) is unique and opens new opportunities for surface engineering and material conversion using heat.In the meantime, nano-tips and cantilevers were further perfected as nanotools to locally induce phase changes in materials for a wide range of exploratory studies. Today, thermal scanning probe lithography (t-SPL) has matured into turn-key systems that can be compared to some extend to electron beam lithography, but without the useof charged particles and without the need for development. The full grasp of potential applications in R&D and production is still growing as the technique is still emerging.

In this talk, we will give first some background how heated AFM probes were initially designed and fabricated that led to today's advanced thermo-mechanical probe design of micro-cantilevers and nano-tips. The paper will then review some main achievements up to date [3] and then present recent results on t-SPL utilized for 2D materials by our own work [4, 5], and will conclude with some outlook on further challenges in hot-tip nanoengineering.

References:

[1] R. Garcia, et al. Nature Nanotechnology (2014)

[2] H. J. Mamin et al. Applied Physics Letters (1992)

[3] S. T. Howell et al. Microsystems & Nanoengineering (2020)

[4] X. Liu et al. Advanced Materials (2020)

[5] X. Liu et al. Nano letters (2020)

10:40am **MN+AS+NS+QS+SE-MoM-8 Atomically-Thin MoS_2 Nanoelectromechanical Resonators**, *R. Yang,* Shanghai Jiao Tong University, China; ***Jaesung Lee,*** University of Texas at El Paso **INVITED**

With the development of the Internet of Things (IoT), new sensors and signal processing elements that consume *near-zero* power to operate on resonance, have high tunability and small form factor are necessary.The ultralow mass and large resonance tunability make resonant 2D nanoelectromechanical systems (NEMS) suitable for ultrasensitive mass, force and biomolecular sensing, radio-frequency (RF) front end, and strain-tunable devices.Further, molybdenum disulfide (MoS_2) resonators only require picowatt level of power for sustaining the strong and stable resonance operations due to their ultralight weight.This opens an opportunity to explore new sensors and signal processing elements for IoT applications that really require near-zero power to operate on resonance, and at the same time, have wide dynamic ranges and tuning ranges. In this talk, we summarize our most recent advances in 2D MoS_2 NEMS resonators.

11:20am **MN+AS+NS+QS+SE-MoM-10 Can a Single Nanomechanical Mode Generate a Frequency Comb?**, ***Eva Weig,*** Technical University of Munich, Germany **INVITED**

Doubly-clamped nanostring resonators excel as high Q nanomechanical systems enabling room temperature quality factors of several 100,000 in the 10 MHz eigenfrequency range. Dielectric transduction via electrically induced gradient fields provides an integrated control scheme while retaining the large mechanical quality factor [1]. Dielectrically controlled nanostrings are an ideal testbed to explore a variety of dynamical phenomena ranging from multimode coupling to coherent control [2]. Here I will focus on the nonlinear dynamics of a single, resonantly driven mode. The broken time reversal symmetry gives rise to the squeezing of the string's fluctuations. As a result of the high mechanical Q factor, the squeezing ratio is directly accessible from a spectral measurement [3]. It is encoded in the intensities of the two spectral peaks arising from the slow dynamics of the system in the rotating frame. For stronger driving, an onset of self-sustained oscillation is observed which leads to the generation of a nanomechanical frequency comb. The effect is a consequence of a resonantly induced negative effective friction force induced by the drive. This is the first observation of a frequency comb arising solely from a single mode and a single, resonant drive tone [4].

[1] Q. P. Unterreithmeier et al., Nature 458, 1001 (2009)

[2] T. Faust et al., Nature Physics 9, 485 (2013)

[3] J. Huber et al., Phys. Rev. X 10, 021066 (2020)

[4] J. Ochs et al., in preparation

Nanoscale Science and Technology Division
Room 304 - Session NS1+QS-MoM

Fabrication, Testing and Metrology of Quantum Devices and Systems

Moderator: Wonhee Ko, Oak Ridge Natinal Laboratory

8:20am **NS1+QS-MoM-1 Single Electrons on Solid Neon: A New Solid-State Qubit Platform with Ultralong Coherence**, ***Xianjing Zhou,*** Pritzker School of Molecular Engineering, University of Chicago **INVITED**

Progress towards the realization of quantum computers requires persistent advances in their constituent building blocks—qubits. Novel qubit platforms that simultaneously embody long coherence, fast operation and large scalability offer compelling advantages in the construction of quantum computers and many other quantum information systems. Electrons, ubiquitous elementary particles of non-zero charge, spin and mass, have commonly been perceived as paradigmatic local quantum information carriers. Despite superior controllability and configurability, their practical performance as qubits through either motional or spin states depends critically on their material environment. In this talk, I will present our experimental realization of a new qubit platform based on isolated single electrons trapped on an ultraclean solid neon surface in vacuum. By integrating an electron trap in a circuit quantum electrodynamics architecture, we achieve strong coupling between the motional states of a single electron and a single microwave photon in an on-chip superconducting resonator [1]. Qubit gate operations and dispersive readout are successfully implemented. Our latest measurements show that both the relaxation time T_1 and coherence time T_2 have reached 0.100-millisecond scale [2]. The observed single-shot readout fidelity, without using a quantum-limited amplifier, is already 94.4%. Simultaneous strong coupling of two qubits with the microwave resonator is also demonstrated, as a first step toward two-qubit entangling gates for universal quantum computing. These results manifest that the electron-on-solid-neon (eNe) charge qubits have outperformed all the existing charge qubits to date and rivaled the state-of-the-art superconducting transmon qubits.

[1] X. Zhou … and D. Jin, "Single electrons on solid neon as a solid-state qubit platform", Nature 605, 46–50 (2022).

[2] X. Zhou … and D. Jin, "Electron charge qubits on solid neon with 0.1 millisecond coherence time", manuscript submitted (2022).

9:00am **NS1+QS-MoM-3 Ultra-thin TaN Damascene Nanowire Structures on 300 mm Si Wafers for Quantum Applications**, ***Ekta Bhatia,*** *S. Kar, S. Olson, T. Vo, S. Schujman, J. Nalaskowski,* NY CREATES; *H. Frost,* SUNY Polytechnic Institute, Albany; *J. Mucci, B. Martinick, I. Wells, T. Murray, C. Johnson, V. Kaushik, S. Papa Rao,* NY CREATES

Tantalum nitride (TaN) is a material which has been used as a copper diffusion barrier in integrated circuits, along with many other applications ranging from corrosion-resistant coatings to superconducting quantum devices. Superconducting nanowire single photon detectors (SNSPDs) are critical for applications in photonic quantum computing, single-flux quantum logic circuits for qubit readout, and neuromorphic computing. TaN SNSPDs have been shown to extend the detection bandwidth to longer wavelengths, along with higher detection efficiency, enabling new applications in cosmology when fabricated into large scale arrays. TaN devices at 300 mm wafer scale can leverage the advances made by the semiconductor industry in process control, improving yield, pattern fidelity and wafer-to-wafer predictability of performance. Hence, the development of this process technology will enable large scale SNSPD arrays, and will also be useful for superconducting circuits for quantum applications.

Detailed studies of the influence of nitrogen content on the superconducting characteristics of TaN thin films are not widely available in the literature, particularly at 300 mm wafer scale. We report the development of ultra-thin reactive sputtered TaN films prepared with different Ta to N ratios on 300 mm scale. We fabricated damascene structures of TaN nanowires with widths varying from 100 to 3000 nm and thickness varying from 5 to 35 nm using 193 nm optical lithography and advanced chemical mechanical planarization.

We confirmed a sigmoidal dependence of TaN sheet resistance on Ta to N ratio, and a decrease in crystallite size (extracted from XRD measurements). The superconductor to insulator transition as a function of Ta to N ratio is reported. We will also discuss the influence of encapsulation of the superconducting wires with metallic TaN and copper. Cu encapsulation can improve contact resistance during measurement, and has implications for thermal conduction along the length of the superconducting nanowire. In contrast, adding an intervening layer of highly disordered metallic TaN between the superconducting TaN and Cu ensures minimal leakage of Cooper-pairs at TaN/Cu interface. We will report the variation of T_c and J_c of TaN nanowires as a function of film thickness, material characteristics, Ta to N ratio and encapsulation.The potential of ultra-thin TaN films at 300 mm scale will be discussed in the context of applications such as on-chip integration for readout of superconducting qubits, in quantum phase slip studies, and large focal-plane detector arrays for cosmology.

9:20am **NS1+QS-MoM-4 Direct Integration of Atomic Precision Devices into a MOS-Compatible Process***, **Jeffrey Ivie**, D. Campbell, A. Leenheer, C. Halsey, E. Anderson, S. Schmucker, D. Scrymgeour, X. Gao, W. Lepkowski, T. Lu, L. Tracy, S. Misra,* Sandia National Laboratories

Atomic precision advanced manufacturing (APAM) of electrical devices, fabricated using hydrogen depassivation lithography in a scanning tunneling microscope, offers a way to explore device physics with the ultimate degree of control. Almost all previous work has focused on exploring applications in quantum physics, particularly with a focus on qubits, using devices operating at cryogenic temperatures. While APAM may benefit applications in microelectronics, such as the strong doping of contacts in scaled transistors, the high temperature surface preparation of APAM generally makes it incompatible with modern metal-oxide semiconductor (MOS) process flows. To leverage significant past investments in CMOS manufacturing and enable a wider application space for APAM devices, demonstration of direct integration of APAM into existing MOS process flows is required.

To enable direct integration of APAM devices, we have established a natural insertion point for APAM processing between Front-end-of-line (FEOL) and Back-end-of-line (BEOL) steps on Sandia's 0.35-micron CMOS node. The insertion point allows for readily accessed device Si through gentle sputtering and thermal annealing, which has a sufficiently crystalline surface critical for APAM delta doping. Integration of the moderate temperature APAM processing step (<600 °C) between high temperature FEOL processing (1000 °C) and before low temperature BEOL processing (<400 °C) maintains the electrical characteristics of both the inserted APAM delta-doped material and the discrete transistors and integrated circuit components from FEOL. Furthermore, accelerated lifetime measurements of APAM wires demonstrate that patterned APAM material is more robust than standard metal features in modern CMOS devices. Establishing the capability of direct integration of APAM into a CMOS process flow opens the door to enhance CMOS transistors with APAM-based processing along with providing wider manufacturing interest. Similarly, implementation of novel APAM-based devices alongside CMOS circuits is a significant discovery platform for microelectronics, neuromorphic computing hardware, or hybrid quantum applications.

This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

9:40am **NS1+QS-MoM-5 Low Thermal Budget PMOS in Low Temperature Epitaxial Silicon***, **Christopher Allemang**, D. Campbell, J. Ivie, T. Lu, S. Misra,* Sandia National Laboratories

Atomic precision advanced manufacturing (APAM) enables deposition of dopants in silicon (Si) with atomic precision and has been exploited to make donor-based qubits. However, understanding the electrical effects of the process tradeoffs in burying the dopants under an epitaxial Si capping layer grown at low temperatures has remained a challenge, both for qubits and for other microelectronics applications. This cap layer can be deposited at the lowest temperatures to limit the diffusion of dopants, or at modest temperatures to limit the density of point defects. Here, to evaluate the electrical quality of the Si cap, we explore using APAM materials and compatible processes for other microelectronic devices, namely p-type metal-oxide-semiconductor (PMOS) field-effect transistors.

The Si cap is unintentionally doped with aluminum during the growth process leading to a p-type material. To employ this p-type material for PMOS, we must have ohmic contacts and a way to gate the channel. Typical processes used for contacting and gating the channel, e.g. implants and thermal oxide, cannot be used here because they are high temperature processes. To maintain an APAM compatible thermal budget, we have developed ohmic contacts to the cap layer using platinum silicide formed at 400ºC and an atomic layer deposition Al_2O_3 gate oxide grown at 250ºC. These temperatures are also within the back-end-of-line thermal budget for Si CMOS, implying this process could be used to integrate an additional device layer on an existing chip.

The silicide contacts are qualified by fabricating Schottky diodes on n-type material and analyzing their current-voltage (*IV*) characteristics, while the gate oxide is qualified by measuring the capacitance-voltage characteristics of MOS capacitors. Further, these processes are combined to demonstrate PMOS transistor behavior in APAM material for the first time. The electrical transport in the cap layer is then qualified using *IV* measurements. While these results represent the initial qualification of electrical transport in the cap layer, further studies and analysis may reveal impacts to APAM quantum devices.

This work was partially funded by the Advanced Manufacturing Office project Big Energy Efficient Transistors, supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories, and performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. The views expressed here do not necessarily represent the views of the DOE or the U.S. Government.

Nanoscale Science and Technology Division
Room 304 - Session NS2+AS+EM+SS-MoM

Quantum Based Sensors and Metrology

Moderator: Nikolai Klimov, National Institute of Standards and Technology

10:40am **NS2+AS+EM+SS-MoM-8 Interfacing Biomolecules with Coherent Quantum Sensors***, **Peter Maurer,*** University of Chicago **INVITED**

Quantum optics has had a profound impact on precision measurements, and recently enabled probing various physical quantities, such as magnetic fields and temperature, with nanoscale spatial resolution. In my talk, I will discuss the development and application of novel quantum metrological techniques that enable the study of biological systems in a new regime. I will start with a general introduction to quantum sensing and its applications to nanoscale nuclear magnetic resonance (NMR) spectroscopy. In this context, I will discuss how we can utilize tools from single-molecule biophysics to interface a coherent quantum sensor with individual intact biomolecules, and how this could eventually pave the way towards a new generation of biophysical and diagnostic devices.

Nanoscale Science and Technology Division
Room 304 - Session NS3+EM+TF-MoM

Nanophotonics, Metasurfaces and Plasmonic Systems Including Inverse Design Methods

Moderators: David Czaplewski, Argonne National Laboratory, **Nikolai Klimov**, National Institute of Standards and Technology

11:20am **NS3+EM+TF-MoM-10 Quantum and Nonlinear Photonics in Silicon Carbide with Inverse Design***, **Daniil Lukin**, J. Vuckovic,* Stanford University **INVITED**

Integrated photonics technology has achieved the degree of scalability and complexity needed for building up photonic quantum computers based on optically-addressable spin qubits such as color centers. However, at present none of the industry-standard photonics materials host high quality color centers. Silicon Carbide has the potential to become a technologically-mature platform that can close this longstanding gap between classical and quantum photonics devices. I will discuss the recent progress of Silicon Carbide integrated photonics for quantum and nonlinear applications, as well as the applications of inverse-design for novel photonics functionalities.

Nanoscale Science and Technology Division
Room 304 - Session NS1+AS+EM-MoA

Correlative Microscopy for Nanoscale Characterization

Moderators: Sidney Cohen, Weizmann Institute of Science, Israel, **Georg Fantner**, EPFL, Switzerland

1:40pm **NS1+AS+EM-MoA-1 Large Volume 3D Biological Imaging with Electron and Cryo-Super-Resolution Microscopy***, **Harald Hess,*** HHMI, Janelia **INVITED**

Volume or 3D electron microscopy continues to expand its potential for imaging ever larger biological entities while preserving a best compromise step edge isotropic resolution of 5-10 nm. This was driven by the challenge of imaging the entire fly brain in sufficient detail for extracting the circuitry of connectome. While the resolution is not of the standards of TEM's, such resolution is of unique value when it encompasses whole cells and complete tissues.We will review the capabilities of FIB-SEM, with ~100 micron sized volumes. Numerous examples can be browsed on openorganelle.com . A cryogenic protocol involving sample vitrification, cryogenic imaging by structured illumination or by photoactivated localization microscopy then followed by staining and resin embedding can then produce the sample suitable for further FIBSEM imaging. This effectively adds protein location information as a color to the 3D EM image. Likewise, several examples correlating specific proteins in the nucleus, on membranes, on and defining organelles and vesicles. Prospects of future challenges are discussed. We will also describe a system capable of imaging volumes approaching 1 mm^3 It is based on Ion Beam Etching and Milling with a Multi beam Scanning Electron MicroscopeIBEaM MSEM.

2:20pm **NS1+AS+EM-MoA-3 The Role of SnO_2 Processing on Ionic Migration in Multi-Halide Perovskites***, **Holland Hysmith,*** University of Tennessee Knoxville*; S. Park,* National Renewable Energy Laboratory*; A. Ievlev, Y. Liu,* Oak Ridge National Laboratory*; K. Zhu,* National Renewable Energy Laboratory*; M. Ahmadi,* University of Tennessee Knoxville*; J. Berry,* National Renewable Energy Laboratory*; O. Ovchinnikova,* Oak Ridge National Laboratory

Moving towards a future of efficient, accessible, and less carbon reliant energy devices has been at the forefront of energy research innovations for the past 30 years. Multi-halide perovskite (MHP) thin films have gained significant attention due to their flexibility of device applications and tunable capabilities for improving power conversion efficiency.[1] Many behavioral aspects to MHP's are thoroughly investigated: functionality of grain boundaries, recombination effects, ionic migration patterns, and hysteresis.[2-4]

Chemical Vapor Deposition (CVD) is a widely used technique for thin film coatings due to its ability for producing high volume batches of MHP's with larger grain sizes, fewer defects, and fewer grain boundary formations.[5-6] Additionally, nanoparticle processing has been applied to induce enlargement of grain boundaries, showcasing larger current signals than its MHP counterparts.[7] Therefore, how does common substrate processing techniques (i.e. CVD, nanoparticles, hybrid) influence the behavior of MHP phenomenon such as ion migration and grain boundary formation? Speculated as inducing ionic recombination and driving I-V hysteresis in MHP's, understanding how chemistry can be tuned to reduce such effects would be optimal.[8-9]

We demonstrate how a hybrid approach of CVD and nanoparticle SnO_2 substrate processing significantly improves the performance of $(FAPbI_3)_{0.97}(MAPbBr_3)_{0.03}$ perovskites in comparison to each technique utilized on its own. As shown in **Figure 1**, higher performing hybrid devices exhibit fused grain boundary formations, not seen in exclusive CVD or nanoparticle devices. Conductive Atomic Force Microscopy (c-AFM) was used to track fused boundary locations and differentiate them from topographic features. Such fusing behavior has been previously observed to showcase higher counts of current and reduce defects such has halide vacancies.[7]

In summary, to understand the chemistry behavior with respect to each device interface, Time of Flight Secondary Ionization Mass Spectrometry (ToF-SIMS) depth profiling was applied. Demonstrated in **Figure 2**, migration of K^+, Na^+, Ca^+, FA^+, MA^+ was found in hybrid devices, in addition to Ca^+ and Na^+ clustering on the perovskite/air layer. Salt clustering could be correlated to the fusing effect demonstrated in the surface morphology imaged in c-AFM. Presence of K^+ has shown to reduce defects driven by alkali iodides like NaI^- and Ca^+ can help with enlarging the bandgap layer in studies where Ca+ was used to replace Pb^+.[10-11] Furthermore, reduced separation between positive ion such as MA^+ and FA^+ from negative ions can decrease the potential responsible for I-V hysteresis.[12]

2:40pm **NS1+AS+EM-MoA-4 Nanoplastic Arrays – from Chaotic Measurements to New Order***, A. Madison, D. Westly, R. Ilic, C. Copeland, A. Pintar, C. Camp, J. Liddle,* ***Samuel M. Stavis,*** National Institute of Standards and Technology (NIST)

Nanoplastic particles are ubiquitous contaminants of the environment, and their unknown hazards are of deepening concern. Optical microspectroscopy is essential to elucidate the structure–property relationships of nanoplastic particles. However, a lack of standards that are fit for purpose limits the reliability of such measurements, resulting in a growing spate of chaotic reports. In particular, the default standard of a colloidal suspension has disadvantages, with sample preparation typically resulting in disordered arrays of nanoparticles with uncontrolled sizes on imaging substrates. Moreover, existing nanoplastic standards can have broad and asymmetric distributions of optical properties. This issue confounds inference of dimensional properties and requires further study.

Optical microspectroscopy often involves contrast from Rayleigh scattering, fluorescence emission, and Raman scattering to detect, quantify, and identify nanoplastic particles. Numerous issues limit accuracy, including optical responses that vary with nanoparticle dimensions and imaging systems that present aberration effects. These issues require standards that provide reference values of dimensional, optical, and positional properties. The latter issue is unexplored, motivating a new order of microscopy standards.

We introduce the concept of the nanoplastic array, addressing these issues. This prototype standard enables calibration, correction, and correlation of image data from multiple instruments, improving the accuracy of microspectroscopy measurements. To prove the concept, we fabricate nanoplastic arrays in nanoscale films of phenolic resin by electron-beam lithography, including both fluorescent dopants and sorbents to study optical properties that are indicators of chemical sorption and resulting hazards.

Our nanoplastic arrays feature three types of nanostructures. The simplest is a uniform film, enabling correction of non-uniform irradiance for the accurate analysis of fluorescence intensity, and providing reference spectra for Raman measurements. Building in complexity, arrays of uniform pillars provide reference dimensions and positions to correlate and calibrate multiple imaging modes. Finally, and most complex, variable pillar arrays facilitate measurements of optical properties as a function of dimensional properties, with fine gradations of pillar diameter enabling quantification of the limits of detection.

Nanoplastic arrays will enable new accuracy and reliability in optical microspectroscopy, advancing the quantitative study of nanoplastic contaminants to transform unknown hazards into known quantities.

3:00pm **NS1+AS+EM-MoA-5 Development of Nanoendoscopy-AFM for Visualizing Intracellular Nanostructures of Living Cells***, **Keisuke Miyazawa,*** Kanazawa University, Japan*; M. Penedo,* EPFL, Switzerland*; N. Okano, H. Furusho, T. Ichikawa, M. Shahidul Alam, K. Miyata,* Kanazawa University, Japan*; C. Nakamura,* AIST, Japan*; T. Fukuma,* Kanazawa University, Japan

Atomic force microscopy (AFM) is the only technique that allows label-free imaging of nanoscale biomolecular dynamics, playing a crucial role in solving biological questions that cannot be addressed by other major bioimaging tools (fluorescence or electron microscopy). However, such imaging is possible only for systems either extracted from cells or reconstructed on solid substrates. Thus, nanodynamics inside living cells largely remain inaccessible with the current nanoimaging techniques. Here, we overcome this limitation by the nanoendoscopy-AFM, where we fabricate a needle-like nanoprobe (diameter < 200 nm, length > 500 nm) made of Sillicon or Carbon, and insert it into a living cell directly in order to measure a force curve, and visualize 2D or 3D internal structures of living cells by the measured 3D force applied to the tip during three-dimensional tip scanning. By using this method, we measured the 3D force image of a human cancer cell (HeLa). The result clearly shows the nucleus in the living cell. In addition, our results using the developed nanoendoscopy-AFM showed undetectable changes by the previous methods such as actin fiber three-dimensional (3D) maps, and 2D nanodynamics of the membrane inner scaffold in the living cells. Unlike previous AFM methods, the nanoprobe directly accesses the target intracellular components, exploiting all the AFM capabilities, such as high-resolution imaging, nanomechanical mapping, and molecular recognition. These features of the nanoendoscopy-AFM should greatly expand the range of intracellular

structures observable in living cells, and contribute to the various life science research fields.

Nanoscale Science and Technology Division
Room 304 - Session NS2+AP+BI-MoA

Fabrication and Operation of Nano-Systems

Moderator: David Czaplewski, Argonne National Laboratory

4:00pm **NS2+AP+BI-MoA-8 Control of Color Centers in Diamond using Photonic and Phononic Crystals**, ***Kazuhiro Kuruma,*** Harvard University **INVITED**

Color centers in diamond are one of the promising solid-state quantum emitters for the realization of on-chip quantum network. In particular, SiV centers have been investigated owing to their optically accessible spins as well as large and stable zero phonon line emission in photonic nanostructures. The integration of the SiV centers into the nanostructures such as photonic crystal nanocavities has been demonstrated as an efficient spin-photon interface for various quantum applications [1]. However, SiV centers need operations at mK temperatures [2] or under static strain [3] to achieve a long spin coherence time. I will show another potential approach using phononic crystals as a way to enable the realization of a long spin coherence time at higher temperatures[4]. Our efforts aimed at efficient control of the SiV spins using diamond optomechanical cavities will also be discussed [5]. Finally, I will present our works on the integration of tin-vacancy (SnV) centers, alternatives to SiV centers for operations at higher temperatures, into free-standing photonic crystal nanocavities [6].

1. M. K. Bhaskar, R. Riedinger, B. Machielse, D. S. Levonian, C. T. Nguyen, E. N. Knall, H. Park, D. Englund, M. Lončar, D. D. Sukachev, and M. D. Lukin, "Experimental demonstration of memory-enhanced quantum communication," Nature 580, 60–64 (2020).
2. D. D. Sukachev, A. Sipahigil, C. T. Nguyen, M. K. Bhaskar, R. E. Evans, F. Jelezko, and M. D. Lukin, "Silicon-Vacancy Spin Qubit in Diamond: A Quantum Memory Exceeding 10 ms with Single-Shot State Readout," Phys. Rev. Lett. 119, 223602 (2017).
3. Y.-I. Sohn, S. Meesala, B. Pingault, H. A. Atikian, J. Holzgrafe, M. Gündoğan, C. Stavrakas, M. J. Stanley, A. Sipahigil, J. Choi, M. Zhang, J. L. Pacheco, J. Abraham, E. Bielejec, M. D. Lukin, M. Atatüre, and M. Lončar, "Controlling the coherence of a diamond spin qubit through its strain environment," Nat. Commun. 9, 2012 (2018).
4. C. Chia, K. Kuruma, B. Pingault, M.. Lončar. "Controlling Coherence Time of Silicon Vacancy Centers in Diamond Using Phononic Crystals." CLEO 2021, FTh4M.2, San Jose, California, May 2021.
5. M. Haas, K. Kuruma, G. Joe, B. Machielse, D. Assumpcao, C. Chia, N. Sinclair, and M. Lončar, "Visible-Wavelength Optomechanical Crystal for Coupling Phonons to a Silicon Vacancy Center in Diamond", CLEO 2022, FW4I.2, San Jose, USA, May 2022
6. K. Kuruma, B. Pingault, C. Chia, D. Renaud, P. Hoffmann, S. Iwamoto, C. Ronning, and M. Lončar, "Coupling of a single tin-vacancy center to a photonic crystal cavity in diamond," Appl. Phys. Lett. 118, 230601 (2021).

4:40pm **NS2+AP+BI-MoA-10 Scalable Preparation of Intrinsically Chiral Metal Surfaces for Enantioselective Processes**, ***Nisha Shukla,*** *A. Gellman,* Carnegie Mellon University, USA

Chiral surfaces are critical components of enantioselective heterogeneous processes such as those used to prepare enantiomerically pure pharmaceuticals. While the majority of chiral surfaces in practical use are based on achiral materials whose surfaces have been modified with enantiomerically pure chiral adsorbates, there are many inorganic materials with valuable surface properties that could be rendered enantiospecific, if their surfaces were intrinsically chiral.

This work discusses recent developments in the fabrication of intrinsically chiral surfaces exhibiting enantiospecific adsorption, surface chemistry and electron emission. We propose possible paths to the scalable fabrication of high-surface-area, enantiomerically pure surfaces and discuss opportunities for future progress.

5:00pm **NS2+AP+BI-MoA-11 Wrinkle-Induced, Scale-Dependent Mechanical Properties in Nanometer Thick Films**, ***Jian Zhou,*** *N. Moldovan, L. Stan, J. Wen, D. Jin,* Argonne National Lab*; D. Lopez,* Pennsylvania State University*; D. Czaplewski,* Argonne National Lab

Micro- and nano-electromechanical (MEMS/NEMS) devices have relied heavily on materials typically used in electronic devices. The majority of MEMS/NEMS devices are fabricated with a top-down approach to take advantage of the corresponding highly reproducible fabrication processes associated with silicon related materials. As a natural extension, as devices move into the nanoscale regime, new materials are introduced using the same fabrication paradigms used for electronics: ultra-flat surfaces, controlled stresses, simply defined materials properties, with precision 2-dimensional or 2+ dimensional definition using lithographic techniques. New materials, such as 2D materials, began to be incorporated with great promise. However, creating 2D material films that behave like traditional silicon-related films has become challenging due to their unconventional growth/deposition techniques. A typical method for depositing a 2D film is through a transfer process, which struggles to create flat, low stress, thin films. This has led to films that have variations in properties, as observed in large deviations in values reported for parameters such as Young's modulus.

In this work, we explore the variation in properties of films as they become more 2+dimensional textured versus being ultra-flat. We measure the response of resonators fabricated from both ultra-flat and wrinkled films. The ultra-flat films follow expected behaviors with small deviations in resonant frequency and bending rigidity. However, the wrinkled films have a frequency response that is highly variable, up to 45 times that found in flat films. Additionally, we find that the increased rigidity and distribution of values is scale-dependent. As we vary the in-plane dimensions of the resonant structures, we find that the characteristic values scale with the structure dimension. This matches very well with a theoretical model proposed to describe thermal fluctuations in thin films. This opens a new paradigm for device design that allows a single film to have multiple elastic properties based solely on the patterning size. Going forward, we see this being an interesting tool in the design of devices made from single nanometer-thick films.

Biomaterial Interfaces Division
Room 318 - Session BI1+AS+EM+NS+SE+TF-TuM

Bioanalytics, Biosensors and Diagnostics

Moderators: Caitlin Howell, University of Maine, **Laura Mears**, TU Wien, Austria

8:00am **BI1+AS+EM+NS+SE+TF-TuM-1 Understanding and Employing Adhesion Forces in Microfluidic Channels for Cell Separation***, Avi Gupta, F. Chrit, A. Liu, A. Alexeev, T. Sulchek,* Georgia Institute of Technology, USA

Rapid advancements in microfluidic technologies during the past few decades have significantly aided advancements in the field of BioMEMS. These technologies can facilitate development of easily scalable tools that can be translated to point-of-care healthcare products. Researchers have capitalized on these tools to create differential separation techniques that rely on adhesion forces. The adhesive interactions play a significant role in governing the trajectory of cells in microfluidic channels as well as the reliability of these devices, however, a concise model explaining cell interactions with chemically coated surfaces is yet to be developed. This research describes studies using microfluidic flow at different flow regimes to study dynamic cell adhesion. APTES, P-selectin, and Pluronic were used as models for non-specific adhesion, specific adhesion, and adhesion-free surfaces, respectively. A microfluidic device with slanting ridges was used to provide forced contact and to visualize the effect of these chemistries on cell trajectories using a microscope and a high-speed camera. Parameters of the channel that were studied include ridge angle, gap size, channel width, and flow rate. It was found that adhesive forces modulate the interaction time of cells during contact points with the slanting ridges. At an average flow velocity of 3.1 cm/sec we observed higher interaction time for APTES coatings and lower for Pluronic coatings. Higher adhesion on APTES coated surface of the channel leads to more deflection of cells towards the streamlines leading them to go opposite to the ridge direction. In contrast, lower surface adhesion on Pluronic coated surface made cells deviate along the ridge perpendicular to streamlines. Narrow channel widths and acute ridge angles helped in exaggerating the differences in trajectories of cells going along or under the ridge. Atomic force microscopy (AFM) was used to quantify the adhesion forces. This knowledge was used to develop a predictive model employing Lattice Boltzmann techniques along with Morse potential and Bell model to represent interaction between cells and device surface. This improved understanding of adhesion forces in microfluidic devices opens new avenues for developing separation techniques that don't employ specific molecules like P-selectin but rely upon the inherent geometry and surface interaction of the cells with a microfluidic channel.

8:20am **BI1+AS+EM+NS+SE+TF-TuM-2 Wafer-Scale Metallic Nanotube Arrays with Highly Ordered Periodicity for SERS Application***, Jinn Chu,* National Taiwan University of Science and Technology, Taiwan

This paper reports on the wafer-scale fabrication of ultrahigh sensitivity SERS substrates using metallic nanotube arrays (MeNTAs) with highly ordered periodicity. Various metals and alloys have been used to prepare MeNTAs via sputtering over a contact-hole array template created in photoresist. These include ferrous (stainless steel) and nonferrous (Cu-, Ni-, Al-, and Ti-based) alloys, as well as elemental metals (Cu, Ag, and Au). The proposed nanotubes can be fabricated over a wide range of heights and diameters (from a few hundred nm to 10 μm) in a variety of shapes, including tall cylinders and dishes. In addition, over this is deposited a uniform coating of Au nanoparticles to form a high-sensitivity AuNP@MeNTAs 3D-SERS substrate. Systematic micro-Raman spectroscopic analysis reveal that the fabricated array could function as a SERS-active substrate with crystal violet (CV) and folic acid as analytes (a minimum detection limit of 10^{-13} M CV). Enhancement factor of 1.06×10^9 is obtained from our triangular Ag MeNTA. This work is the first to fabricate wafer-scale metallic nanotube arrays with SERS properties, which represents an important step toward realizing the large-scale fabrication of ultrasensitive SERS-active materials.

8:40am **BI1+AS+EM+NS+SE+TF-TuM-3 Customizing Silk Film Surface Properties Using Plasma-Enhanced Chemical Vapor Deposition***, A. Devore, G. Reyes, Morgan Hawker,* California State University, Fresno

Silk fibroin (silk) is a naturally-derived polymer with high utility in biomedical contexts, notably in tissue engineering. Silk bulk properties can be tuned to mechanically match a range of biological environments, including soft and hard tissues. As with other naturally-derived polymers, silk constructs degrade via surface-mediated enzymatic hydrolysis into non-toxic amino acid byproducts. Because tissue engineering relies on the underlying scaffold to degrade as the healthy tissue forms, controlling silk scaffold degradation kinetics is essential to maximize silk's utility. Notably, prior work to control silk degradation kinetics relies on either altering silk matrix properties (i.e., manipulating the secondary structure), or through creating silk-containing blends such as copolymers. Although both strategies effectively control degradation, doing so is often at the expense of mechanical properties. Any mechanical mismatch induced through controlling degradation can hinder scaffold function. Developing a strategy to program silk degradation - without altering bulk mechanical properties - is required to enhance their efficacy as biomaterials.

This talk will highlight recent efforts to develop a radio-frequency plasma-enhanced chemical vapor deposition (PECVD) approach with the potential to modulate silk degradation. The long-term objective of this work is to control the rate of surface-mediated enzymatic hydrolysis by customizing silk surface properties. Surface properties are thought to be paramount in controlling silk construct/enzyme interactions, so tuning silk film surface properties using PECVD was a logical first step. Silk films were first dropcasted, and were then subjected to PECVD. Plasma feedgas composition was tuned using two unique precursors: acrylic acid (to produce thin films with polar functional groups on the silk surface), and pentane (to produce thin films with non-polar functional groups on the silk surface). Plasma polymerization using mixed precursor conditions was also explored. Contact angle goniometry was utilized to evaluate the wettability of all plasma-modified and control silk films. Changes in surface chemistry were evaluated using high-resolution x-ray photoelectron spectroscopy. Collectively, findings demonstrated that surface properties depend on both feedgas composition and position of the silk film in the plasma reactor. In sum, PECVD represents a promising approach to customize silk surface properties.

9:00am **BI1+AS+EM+NS+SE+TF-TuM-4 Biopotential Sensing Using Flexible, Reusable Smart Textile-Based Dry Electrodes***, Jitendra Pratap Singh,* Physics Dept IIT Delhi, India

Biopotential signals are used to assess organ function and make diagnoses. Biopotential electrodes are used to monitor and record biopotentials by acting as an interface between biological tissue and electrical circuits. The accurate detection of physiological signals from the human body is essential for health monitoring, preventive care, and treatments.

Wearable bioelectronics developments applied directly on the epidermal surface provide a promising future biopotential sensing option. Wearable textile electrodes for biopotential sensing are a promising candidate for long-term health monitoring. Wearable health-monitoring devices should be simple to use, stigma-free, and capable of delivering high-quality data. Smart textiles, which incorporate electronic elements directly into the fabric, offer a seamless way to incorporate sensors into garments for a variety of purposes. This work describes different types of flexible and reusable textile-based dry electrodes for biopotential monitoring. This work also describes the direct writing of laser-induced graphene (LIG) on a Kevlar textile for the production of reusable dry electrodes for long-term ECG monitoring. The electrode as-prepared has a high electrical conductivity and skin contact impedance of 100 ± 1 kΩ to 7.9 ± 2.7 kΩ for frequencies ranging from 40 Hz to 1 kHz, which is comparable to conventional Ag/AgCl wet electrodes.

The outcomes demonstrate comparable performance with significantly reduced electrode-skin impedance for clinical-grade devices. Even after several hours of usage, these electrodes do not irritate the skin and are effective without any skin preparation. As a result of their flexibility and a better match to the modulus of the skin, it is anticipated that the suggested dry electrodes will provide comfort for long-term biopotential monitoring. A simple, cost-effective, and scalable fabrication approach enables the fabrication of flexible electrodes of arbitrary shape for long-term biopotential monitoring.

1. Y. Maithani, B. Choudhuri, B. R. Mehta, and J. P. Singh: Self-adhesive, Stretchable, and Dry Silver Nanorods Embedded Polydimethylsiloxane Biopotential Electrodes for Electrocardiography. *Sensors Actuators A Phys.***332**, 113068 (2021).
2. Y. Maithani, B. Choudhuri, B. R. Mehta, and J. P. Singh: Modelling and Analysis of Active Biopotential Signals in Healthcare , Volume 2 A comprehensive review of the fabrication and performance evaluation of dry electrodes for

long - term ECG monitoring. *IOP Publ. Ltd 2020***2**(chapter 8), 1 (2020).

9:20am **BI1+AS+EM+NS+SE+TF-TuM-5 Functional Plasma Polymers for Biosensing Applications***, **Melanie McGregor,*** University of South Australia **INVITED**

Materials with intricate nanostructures display wetting properties that modern technologies already use to lubricate engines or waterproof clothing. Yet, their full potential in applications for sustainable catalysis, air purification or biosensing cannot be realised until we understand how nano-objects adsorb to surfaces with features of comparable size. Indeed, controlling or even predicting how proteins, antibodies, exosomes, surfactant or nanoparticles stick to nano-engineered surfaces is a challenge because key aspects of the wetting phenomenon remain poorly understood at this scale. In this talk, I will briefly review what we currently know about "nanowetting".[1] I will then introduce the concept of plasma polymerisation as a technique to control both surface chemistry and surface topography. I'll use the example of plasma deposited polyoxazoline (POx) to highlight this technique's attributes, drawbacks and recent progress made in understanding the unique chemistry and reactivity of POx films, using both plasma in-situ and post deposition spectroscopic analysis.[2]Plasma deposited Polyoxazoline thin films share many valuable properties with polyoxazoline prepared via conventional organic chemistry: they are biocompatible, non-cytotoxic and low fouling.[3] What is more, they bind biomolecules covalently, support cell adhesion, and are generated in a solvent free, single step process, which makes them particularly attractive for industrialization. For these reasons, plasma deposited polyoxazoline are used in applied biomedical research, from in vitro stem cell culture to controlling immune responses.[4]

I'll conclude this presentation with tangible outcomes of the translational research projects I've conducted with various industries, where we used nanoengineered plasma polymers, to create materials for cancer diagnosis and growing organoids.[5]

[1]**M. MacGregor** and K. Vasilev. *Advanced Materials Interfaces,4*, 1700381.,2017**;M. MacGregor** et al., *Nanoscale*, 8(8),4635-4642, 2016

[2] **M. Macgregor***et al.*Chemistry of Materials, 29(19)8047-51,* 2017; **M. N. MacGregor**-Ramiasa et al., *J. Mat. Chem. B*, 3, 6327-6337, 2015

[3]**M. N. Ramiasa** et al. *Chem. Commun.*, 51, 4279-4282,2015**;**A. A. Cavallaro, **M. N. Macgregor**-Ramiasa, K. Vasilev, *ACS Appl. Mater. Interfaces8*, 6354, 2016.

[4] R. M. Visalakshan, A. A. Cavallaro, **M. N. MacGregor**, et al. *Adv. Funct. Mat.*, 29, 1807453, 2019**;**

[5]**M. MacGregor***et al. *Biosensors and Bioelectronics,* 171: 112699,2020; K.M. Chan […]**M. MacGregor****Cancers* 13(21), 5544 2021

Mini Symposium on 2D Materials Synthesis
Room 303 - Session MS-2DMS+2D+EM+NS-TuM
Direct Growth of 2D Materials, Including CVD and MBE

Moderators: Matthias Batzill, University of South Florida, **Erica Douglas**, Sandia National Laboratories, **Maryam Ebrahimi**, Lakehead University, Canada, **Kathleen McCreary**, Naval Research Laboratory

8:00am **MS-2DMS+2D+EM+NS-TuM-1 Efficient Control of 2D Magnetism***, **Cheng Gong,*** University of Maryland **INVITED**

The recently discovered magnetic two-dimensional (2D) van der Waals materials [1, 2] provide ideal platforms to enable the atomic-thin, flexible, lightweight magneto-optical and magnetoelectric devices. Though many have hoped that the ultra-thinness of 2D magnets should allow an efficient control of magnetism, the state-of-the-art has not achieved notable breakthroughs to this end, with only proof-of-concept reports. There appear to be some fundamental obstacles for efficient control. In this talk, I will analyze the challenges and present our recent theoretical and experimental progress on efficient electrical and optical control of 2D magnetism [3-7]. We envision the efficient control of 2D magnets could open new avenues for the low-power spintronics and photonics.

1. C. Gong et al. Nature 546, 265-269 (2017).
2. C. Gong, X. Zhang. Science 363, eaav4450 (2019).
3. C. Gong, et al. Nature Communications 10, 2657 (2019).
4. S.-J. Gong, et al. PNAS 115, 8511-8516 (2018).
5. E.-W. Du, et al. Nano Letters 20, 7230-7236 (2020).
6. T. Xie, et al. under review (2022).
7. S. Liang, et al. under review (2022).

8:40am **MS-2DMS+2D+EM+NS-TuM-3 Epitaxial Growth of Transition Metal Dichalcogenide Monolayers for Large Area Device Applications***, J. Redwing, **Thomas V. Mc Knight,*** The Pennsylvania State University **INVITED**

Wafer-scale epitaxial growth of semiconducting transition metal dichalcogenide (TMD) monolayers such as MoS_2, WS_2 and WSe_2 is of significant interest for device applications to circumvent size limitations associated with the use of exfoliated flakes. Epitaxy is required to achieve single crystal films over large areas via coalescence of TMD domains. Our research has focused on epitaxial growth of 2D semiconducting TMDs on c-plane sapphire substrates using metalorganic chemical vapor deposition (MOCVD).Steps on the miscut sapphire surface serve as preferential sites for nucleation and can be used to induce a preferred crystallographic direction to the TMD domains which enables a reduction in twin boundaries in coalesced films. The step-directed growth is dependent on the surface termination of the sapphire which can be altered through pre-growth annealing in H_2 and chalcogen-rich environments. Uniform growth of TMD monolayers with significantly reduced inversion domains is demonstrated on 2" diameter c-plane sapphire substrates enabling large area transfer of monolayers for characterization and device fabrication and testing.Applications for wafer-scale TMD monolayers in nanoelectronics, sensing and photonics will be discussed.

9:20am **MS-2DMS+2D+EM+NS-TuM-5 Formation of Transition Metal Dichalcogenide Janus Monolayers and 2D Alloys Through Non-Equilibrium Synthesis and Processing Approaches***, **Kai Xiao**, S. Harris, Y. Lin, C. Liu,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; G. Duscher,* University of Tennessee Knoxville*; M. Yoon,* Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*; L. Liang, C. Rouleau, A. Puretzky, D. Geohegan,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Doping and alloying in 2D materials are efficient ways to tune the optical and electronic properties, induce new crystal structures and phases, and add new functionalities. In this talk, I will introduce how to precisely tailor the doping of 2D TMDs using non-equilibrium synthesis and processing techniques including chemical vapor deposition and hydrothermal laser implantation. By tailoring isoelectronic doping of chalcogens and metals in 2D TMDs (e.g., $MoSe_2$, WS_2) during CVD synthesis, the uniform alloys, gradient alloys, and lateral heterostructures are controlled grown on substrates which exhibit many novel properties including tunable bandgaps, enhanced photoluminescence, modulated charge carriers, etc. I will also describe a novel PLD approach with in situ diagnostics such as Raman and photoluminescence to sensitively tune the kinetic energies of Se clusters (3-5 eV/atom) to selectively implant Se atoms within monolayer WS_2 and MoS_2 crystals to form novel Janus WSSe and MoSSe monolayers. Synthesis science was supported by the U.S. Dept. of Energy, Office of Science, Materials Science and Engineering Division. This work was performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

9:40am **MS-2DMS+2D+EM+NS-TuM-6 Effects of Deposition Technique on Monolayer MoS_2 and WS_2***, **Ama Agyapong,*** *S. Mohney,* Pennsylvania State University

It is important to understand how the deposition of metal contacts affects two-dimensional transition metal dichalcogenides (TMDs) so that we can successfully integrate TMDs into next-generation electronic and optoelectronic devices. This study employs Raman spectroscopy as a non-destructive method to probe structural changes induced by depositing metals on monolayer MoS_2 and WS_2. Differences between electron-beam evaporated and DC magnetron sputtered metal/MoS_2 and metal/WS_2 samples were observed in Raman spectra obtained through a transparent substrate using a backside geometry. The disappearance of characteristic Raman modes of the TMDs indicates structural disorder, as observed for sputtered In, Pd, and Pt films on both monolayer MoS_2 and WS_2. This disorder is introduced even though the metals are not reactive with the TMDs. On the other hand, Raman modes remain if the metals are e-beam evaporated. The mass of the metal atoms appears to impact the structural disorder caused by sputtering, as characteristic MoS_2 and WS_2 modes are preserved (albeit with some changes to the spectra) when lighter metal atoms (Cu and Al) are sputtered. The results of this work provide insight on structural changes at the metal/TMD interface that may not be easily detectable in bulk TMDs, and we conclude that e-beam evaporation is a

less destructive deposition technique for forming metal contacts on 1L TMDs than sputtering.

11:40am **MS-2DMS+2D+EM+NS-TuM-12 The Growth of $Nb_{1+x}Se_2$ by Molecular Beam Epitaxy**, ***Peter Litwin***, *S. Jaszewski, J. Ihlefeld, S. McDonnell,* University of Virginia

$NbSe_2$, a metallic transition metal dichalcogenide, has been the focus of numerous recent scientific studies due to the coexistence of superconductivity and charge density wave states it exhibits at low temperature. While less studied, this material also exists in a metal rich, Nb-intercalated (self-intercalated) phase in which additional Nb atoms populate the van der Waals gap. The self-intercalated phase, $Nb_{1+x}Se_2$, has been studied in the bulk form since the 1960's when it was synthesized by chemical vapor transport techniques; however, thin film synthesis of this material is rarely reported. Here we report on the growth of few layer $Nb_{1+x}Se_2$ by molecular beam epitaxy (MBE). We demonstrate that the degree of Nb-intercalation can be tuned through alteration of the Se to Nb flux ratio used during growth. Interestingly, we find that Nb-intercalation exists in all multilayer films, even under Se to Nb flux ratios as high as 45,000:1. The presence of Nb-intercalation results in an expansion of the material's c-axis lattice parameter which we measure using ex-situ x-ray diffraction (XRD). Chemical analysis of the grown thin films is carried out using in-situ x-ray photoelectron spectroscopy (XPS) and further confirms the Nb-rich nature of the grown thin films. The in-plane electrical conductivity is measured using a 4-point probe measurement tool and shows an inverse relationship with the Se to Nb flux ratio used during growth. Lastly, we also report on the thickness scaling of the material's electrical conductivity down to few-layer thick $Nb_{1+x}Se_2$ thin films.

12:00pm **MS-2DMS+2D+EM+NS-TuM-13 Formation of 1D and 2D Carbon-Based Nanomaterials on Surfaces**, ***Maryam Ebrahimi***, Lakehead University, Canada

On-surface reactions offer a platform to design molecular-based low-dimensional nanomaterials whose chemical and electronic properties can be tailored by their chemical structure. The molecules' functional groups and the reactivity of the substrates control the molecule-molecule and molecule-substrate interactions, which steer the design of the obtained molecular structures.We present various surface reactions for creating 1D and 2D polymers, metal-organic networks, and organometallic structures on Au(111), Ag(111) and Cu(111).To identify their topography and chemical nature, we employ scanning tunnelling microscopy and non-contact atomic force microscopy, and other surface characterization techniques, such as X-ray photoelectron spectroscopy, complemented with density functional theory calculations.

The chemical and thermal stability and structural design of these molecular-based low-dimensional nanomaterials make them promising candidates for various applications. These materials are tailored to exhibit unique electronic properties, charge mobility and/or electron spin-based structure, suitable for carbon-based nanoelectronics, spintronics, and quantum technology applications.

References

[1] M. Ebrahimi, *Nat. Chem.* 14 (2022) 3-4

[2] M. Ebrahimi, F. Rosei, *Nature* 542 (2017) 423-424

[3] M. Ebrahimi, F. Rosei, *Nat. Photonics* 10 (2016) 434-436

[4] G. Galeotti et al., *Nat. Mater.* 19 (2020) 874-880

[5] G. Galeotti et al., *Faraday Discuss.* 204 (2017) 453-469

[6] F. De Marchi et al., *Nanoscale* 10 (2018) 16721-16729

[7] G. Galeotti et al., *Chem. Sci.* 10 (2019) 5167-5175

[8] C. Jing et al., *Angew. Chem. Int. Ed.* 58 (2019) 18948-18956

[9] P. Ji et al., *Small* 16 (2020) 2002393

[10] N. Cao et al., *Nanoscale* 13 (2021) 19884-19889

Plasma Science and Technology Division
Room 305 - Session PS1+NS-TuM

Advanced Plasma Patterning: EUV-Based, Multipatterning and Alternative Patterning Approaches (Imprint, DSA, Etc.)

Moderators: Yohei Ishii, Hitachi High Technologies America Inc., **Angelique Raley**, TEL US

8:00am **PS1+NS-TuM-1 EUV Patterning: Plasma Processing Innovations for Single Exposure and Multi-Patterning**, ***Katie Lutker-Lee***, TEL Technology Center, America, LLC **INVITED**

As extreme ultraviolet (EUV) lithography progresses to a mature high volume manufacturing technology, innovations are still required to meet the device scaling and performance requirements. While many of these innovations may take the shape of integration changes, plasma processing will still play an important role in shaping the next generation of technology. In order to advance plasma processing for the next nodes, we must start looking at plasma process development beyond the standard process tuning knobs. New chemistries and techniques must be thoroughly investigated and out of the box thinking must be applied. The applications to which plasma processing can benefit single exposure and multi-patterning techniques are vast, ranging from roughness and profile improvements to the enablement of new integrations techniques.

In this presentation, we will discuss a few of the many innovations we have investigated to overcome the challenges of EUV patterning. It is well known that EUV lithography suffers from stochastically driven defectivity, in particular, feature breaks and bridges, and high roughness.[1] Plasma based process improvements, including etch process co-optimization with films, and selective deposition, have provided critical improvements in this area.[2,3] Processes such as selective deposition also open the door for innovative integration schemes that would otherwise be inhibited.[4] The advent of high-NA EUV lithography will present its own unique challenges, including new materials, in particular metal containing resists, and even smaller feature sizes, in addition to the known challenges of the current generation of EUV lithography.[5] Advanced plasma processing, especially etch, will play an important role in overcoming these hurdles.

1. L. Meli, J. Church, A. De Silva, K. Petrillo, D. Goldfarb, S. Stieg, R. Lallement, D. Lea, M. Burkhardt, N. Felix, and C. Murray, Proc. SPIE, 116090P (2021).
2. L. Meli, K. Petrillo, A. De Silva, J. Arnold, N. Felix, C. Robinson, B. Briggs, S. Matham, Y. Mignot, J. Shearer, B. Hamieh, K. Hontake, L. Huli, C. Lemley, D. Hetzer, E. Liu, K. Akiteru, S. Kawakami, T. Shimoaoki, Y. Hashimoto, H. Ichinomiya, A. Kai, K. Tanaka, A. Jain, H. Choi, B. Saville, and C. Lenox, J. Micro/ Nanolith. MEM MOEMS, 18, 011006, (2019).
3. J. Church, K. Lutker-Lee, L. Meli, E. Miller, and A. Raley.AVS (2021).
4. K. Lutker-Lee, E. Richardson, D. O'Meara, and A. Raley, Proc. SPIE, 11615, (2021).
5. Thiam, J. G. Santaclara, J-H. Franke, F. Schleicher, R. Blanc, P. Bezard, A. Moussa, P. Wong, E. Hendrickx, and M. J. Maslow, Proc SPIE, 118540A (2021).

8:40am **PS1+NS-TuM-3 Reduction of EUV Resist Damage by using Neutral Beam Etching**, *N. Soo,* School of Advanced Materials Science and Engineering, Sungkyunkwan University, Republic of Korea; ***Geun Young Yeom***, School of Advanced Materials Science and Engineering, Sungkyunkwan University / SKKU Advanced Institute of Nano Technology (SAINT), Sungkyunkwan University, Republic of Korea

Even though Extreme Ultra Violet (EUV) lithography has the advantage of implenting a finer pattern compared to ArF immersion lithography due to the use of 13.5 nm instead of 193 nm as the wavelengh of the light source, due to the low energy of EUV light source, EUV resist has a thinner thickness than conventional ArF resist and it is more vulnerable to radiation damage received during the etching because of its low etch resistance and also tends to have a problem of low etch selectivity. In this study, the radiation damage to an EUV resist during the etching of hardmask materials such as Si_3N_4 and SiO_2 using a CF_4 neutral beam has been investigated and the results were compared with those etched by a CF_4 ion beam. The results showed, for the etching of the same EUV resist thickness, less line edge roughness, less critical dimension loss, and higher etch selectivity to the hardmask materials such as SiO_2 and Si_3N_4 were obtained for the CF_4 neutral beam etching compared to the CF_4 ion beam etching.

Key word : extreme ultraviolet (EUV) lithography, extreme ultraviolet (EUV) PR, low damage, line edge roughness (LER), critical dimension (CD), neutral beam etching(NBE), ion beam etching(IBE)

9:00am **PS1+NS-TuM-4 Numerical Investigation of EUV Induced H_2-O_2 Plasmas and Surface Chemistry**, ***Tugba Piskin,*** University of Michigan*; V. Volynets, S. Nam,* Mechatronics Research, Samsung Electronics Co., Ltd, Republic of Korea*; H. Lee,* Mechatronics Research, Samsung Electronics Co., Ltd., Republic of Korea*; M. Kushner,* University of Michigan

Extreme Ultra-Violet (EUV) systems achieve smaller feature sizes in microelectronics processing by deploying photons with ~10 nm wavelength for photolithography. There are several advanced techniques for generating EUV photon beams; one of which is ablating and ionizing tin droplets with pulsed lasers. Excited tin ions emit photons with a 13.5 nm wavelength. These photon beams are collected and focused with a collector mirror, and then photons are transferred to the scanner unit. The lifetime and reflectivity of the collector mirror decline with time due to deposition of tin. An in-situ cleaning technique of tin deposited on the optics involves pumping H_2 into the chamber. H_2 gas does not substantially attenuate the EUV beams, but the photons have enough energy (92 eV) to create an H_2 plasma through photoionization and photodissociation reactions. Hydrogen radicals then etch the tin deposits by producing stannane, a volatile gas which can be pumped from the chamber. The most significant loss mechanism for hydrogen radicals is recombination reactions on the walls. The addition of a small amount of oxygen helps decrease the wall losses of hydrogen radicals by production of the water vapor. The water vapor adsorbs on surface sites, which blocks recombination of H atoms.

In this paper we discuss results from a computational investigation of the low-pressure H_2-O_2 plasma produced from EUV photon beams in a generic EUV photolithography tool using the Hybrid Plasma Equipment Model (HPEM). The densities of radicals, ions, and excited species, their fluxes (including energy-and-angular distributions) to the chamber walls, and the surface coverage fractions will be discussed. For pressures of a few to tens of Pa and hundreds of Watts EUV power, the addition of oxygen increases hydrogen radical density in the chamber and decreases the surface loss of hydrogen radicals. The consequences of oxygen fraction, pressure, and photon intensity on plasma properties and surface mechanisms will be discussed.

Work supported by Samsung Electronics and the National Science Foundation.

9:20am **PS1+NS-TuM-5 Modeling of Shallow Trench Isolation Etch in Self-aligned Double Patterning Process**, ***Shuo Huang,*** *P. Panneerchelvam, C. Huard,* KLA Corporation*; S. Sridhar, P. Ventzek,* Tokyo Electron America*; M. Smith,* KLA Corporation

As the critical dimensions (CDs) decrease to a few nanometers while the aspect ratios increase beyond 100, the cost of process development significantly increases and the performance of the plasma etch process is critical to the success of ramping a new technology node toward profitable high-volume manufacturing. In this paper, a plasma dry etch simulator developed at KLA, ProETCH® [1], has been applied to investigate a defect that arises in an overlay metrology target in DRAM during shallow trench isolation (STI) etch patterned using self-aligned double patterning (SADP). SADP process is characterized by performing lithography at a pitch that is two times larger than the desired pitch and is followed by spacer deposition, a spacer etch-back and core etch processes. A challenge of this scheme is that each process introduces some non-uniformity, leading to variations in, for example, the hard mask that is eventually utilized for the final etch. One typical defect is the pitch walk, which manifests different trench openings between the pillars. This periodicity is indicative of the SADP process and corresponds to where the resist core line is patterned initially. The principal objective of this work is to investigate the influence of hard mask irregularities on the STI etch process evolution ProETCH. The mechanism of silicon etch by Ar/Cl_2 plasma was developed with the experimental data (cross-section SEM images) as reference. The variations in the hard mask that arise during the SADP process were found to have a significant impact on the printability of these targets. The differences in trench openings result in aspect ratio dependent etch (ARDE), which could be mitigated by modulating the plasma fluxes to the surface.

[1] P. Panneerchelvam et al., Trilayer hard mark lithography and etch for BEOL manufacturing, SPIE Advanced Lithography, San Jose, California, USA, April 2022.

9:40am **PS1+NS-TuM-6 Polymer Engineering for High Aspect Ratio Plasma Etching Enabled by Chemistry**, ***Phong Nguyen,*** *S. Biltek, X. Guo, N. Nathan Stafford,* American Air Liquide

High aspect ratio (HAR) ONON channel etch is a very complex and challenging step in 3DNAND flash memory production and the challenges increase with increasing vertical stack height and reducing pitch sizes. A variety of fluorocarbon gases are used to etch the alternating layers of SiO2 and SiN selective to the mask while maintaining a vertical profile. Control of sidewall polymer formation and its properties such as electrical conductivity are potential pathways to overcome undesirable patterning feature distortions such as bowing, twisting, tilting, and sidewall electrostatic interference i.e “charging.”

We demonstrate that engineering the polymer for both its composition as well as conductivity can be accomplished by modification of the chemistry mixture that is used in the plasma process. Characterization of the polymer is done using XPS, SEM, EDS, and current-voltage (I-V) measurements in a variety of simplified test structures to elucidate the properties of the polymer on the etch front and the sidewall. Understanding of the composition of polymers from standard fluorocarbon chemistries including C4F8 and C4F6 along with new fluorocarbons gases will be presented showing changes in the C/F ratio of the polymer on the sidewall at different aspect ratios as well as the difference in polymer between the etch front and the sidewall of test structures. In addition, Quadrupole Mass Spectrometry (QMS), a powerful tool, is implemented to identify positive ion fragments that might be present inside the plasma. Furthermore, such details can elucidate the deposition and etching characteristic of these ions during HAR etching. The combination of polymer characterization and analysis of gas species via QMS can give us a better understanding of the etching process. Finally, new work in improvement of the polymer conductivity using new etching gases will be presented demonstrating >100x improvement in the polymer conductivity.

11:00am **PS1+NS-TuM-10 Achieving Better Etching Performance with Lower GWP Gases**, ***Nicolas Gosset,*** *T. Hasegawa, V. Gamaleev,* Air Liquide Laboratories, Japan **INVITED**

Nowadays, new architectures and structures for advanced Logic and Memory devices come with new etching processes and challenges. Among them, anisotropic etching of Si dielectric layers with very high selectivity to the mask, defect free soft-landing to the under layers, and profile control (no bowing, twisting, scalloping, clogging, loss in critical dimensions, and etch stop) is needed for the realization of advanced patterns (e.g. gate spacers, SADP, SAQP, high aspect ratio ONON and contact holes). These layers, such as SiO_2 and SiN, are standardly etched using fluorocarbon-based plasmas that involve multiple simultaneous reactions and phenomena. A key one is passivation, used to suppress lateral etching and damages. Etchants such as CF_4, C_4F_8, C_4F_6, CHF_3, CH_3F, etc. allows the etching of SiO_2 and SiN through the generation of mixed and polymer layers which, assisted by ions bombardment, lead to desorption of volatile byproducts such as CO_x, COF_x, SiF_x, NH_x and HCN. Same polymers generated by these standard gases are also used to protect structure’ sidewalls during the etching, where the contribution of ion bombardment is much weaker. Nevertheless, the lack of polymer conformality on the sidewall and its different interactions with the mask or under layer materials strongly contribute to the appearance of etching defects that need to be mitigated.

To mitigate these drawbacks, we investigated the potential of new hydrofluorocarbons-based gases for the etching of high aspect ratio structures, such as 3D NAND holes or DRAM pillars, as well as gate spacers. Not only do these new etchants outperform the ones currently used (higher selectivity to the mask, better profile control, etc.) but they are also more environmentally friendly with lower Global Warming Potentials (GWP). In-depth studies (e.g. polymer deposition, composition, OES, etc.) have shown that these improved performances are linked to the unique polymerization properties of the molecules on the mask and structure sidewalls. The observed differences in profiles etched by two isomers demonstrate the importance and impact not only of the chemical composition but also the molecule structure and design on etch performances. In this example, a first isomer leads to more polymer deposition on the bottom of HAR holes, while polymer generated by a second isomer deposits more on the top. A second example, using a similar approach, demonstrates how the usage of new hydrofluorocarbons in Plasma-Enhanced Atomic Layer Etching process allow reducing SiN spacers footing with a soft-landing on Si channel. Utilizing these lower GWP gases lead to a process with better profile control and similar throughput.

11:40am **PS1+NS-TuM-12 Etch Profile Control for High-Aspect-Ratio Amorphous Carbon Mask Layer Etching**, ***Du Zhang***, *S. Chang, P. Luan, M. Wang,* TEL Technology Center, America, LLC

The etch profile control for the amorphous carbon layer (ACL) is an important step for the 3D NAND fabrication process. Because ACL is the mask material for defining the pattern of the high-aspect-ratio-contact (HARC) dielectric ONON layer etch process, the precise control of its etch profile is necessary. Specifically, an ideal ACL mask profile should be free of symptoms such as hole circularity distortion, profile twisting, bowing, and undercutting. In order to achieve this desired etch performance, knowledge of various etch contributing factors must be systematically derived and applied, including etch surface chemistry, high-aspect-ratio (HAR) etchant transport, ion flux and ion energy angle distribution function (EADF) control, etc.

In this work, we investigate the ACL etch fundamental characteristics through combined 2D chamber-scale plasma simulations with the hybrid plasma-equipment model (HPEM) and 3D etch profile simulations with the Monte-Carlo Feature Profile Model (MCFPM) for an inductively-coupled-plasma (ICP) reactor with RF bias (detailed descriptions of the simulation tools are discussed in M. Wang and M. J. Kushner. J. App. Phys. 107, 023309 (2010)). In particular, we focus on the profile trends under different reactant fluxes and energies. Our findings indicate that maintaining a neutral-starved (ion-rich) etch regime is essential for the mitigation of both the channel hole etch circularity distortion and the slit etch profile twisting. To achieve this desired etch regime, the HAR ion and neutral transport must controlled by the RF bias power and frequency, substrate temperature, etc. Furthermore, especially in this neutral-limited etch regime which is necessary for distortion and twisting mitigation, the control of the consequent aspect-ratio dependent etching (ARDE) as well as maintaining the critical dimension (CD) and reducing bowing and undercutting are also necessary. For this purpose, atomistic density functional theory (DFT) calculations have been applied to compare the reaction energetics for various ALD-like sidewall passivation chemistries. Specifically, we propose a new process based on its favorable reaction energetics. Experimental cross-section images have matched simulation results. In conclusion, our insights have provided guidance for process optimization and tool design to meet the industrial demands.

12:00pm **PS1+NS-TuM-13 A Mask-free and Contactless Plasma Patterning Technique for Interdigitated Back Contact Silicon Heterojunction Solar Cells Fabrication**, ***Junkang Wang***, *M. Ghosh, P. Bulkin, D. Daineka, P. Roca i Cabarrocas,* LPICM-CNRS, École Polytechnique, Institut Polytechnique de Paris, France*; S. Filonovich,* TotalEnergies GRP, France*; J. Alvarez,* Laboratoire de Génie Electrique et Electronique de Paris, CNRS, CentraleSupélec, Université Paris-Saclay, France*; E. V. Johnson,* LPICM-CNRS, École Polytechnique, Institut Polytechnique de Paris, France

Benefiting from the interdigitated back contact (IBC) architecture and the silicon heterojunction (SHJ) technology, IBC-SHJ solar cell currently holds the record efficiency for single-junction solar cells based on crystalline silicon [1]. However, the necessity of performing photolithographic patterning steps to form the interdigitated carrier collection zones makes this architecture unsuitable for low-cost, high-throughput manufacturing processes.

We present here a novel method that allows the creation of the interdigitated carrier collection zones for IBC-SHJ solar cells by PECVD process in a maskless and contactless manner. This method involves using a slottedpowered RF electrode, which has parallel slits in it, in a custom-designed CCP-PECVD chamber. By keeping the RF electrode in close proximity to the substrate surface (down to sub-mm range), plasma will selectively light only within the slits, thus mimicking the patterns on the electrode [2]. Deploying this patterned plasma process with an etching gas mixture (NF_3/Ar) on a well-designed silicon thin film stack, the interdigitated carrier collection zones required for an IBC architecture have been obtained.

Multiple structural and electrical characterizations (profilometry, spectroscopic ellipsometry, photoluminescence, photovoltage mapping, and secondary ion mass spectroscopy) are performed throughout the whole process flow, which gives good guidance for the processes optimization. The J(V) characteristics of the solar cells fabricated by this method will be presented, and the importance of an additional step to remove the damaged layer on the surface left by the patterned etching process will also be discussed.

References

[1] K. Yoshikawa, et al., “Silicon heterojunction solar cell with interdigitated back contacts for a photoconversion efficiency over 26%”, Nat. Energy, 2, 17032 (2017).

[2] R Léal, et al., “Maskless and contactless patterned silicon deposition using a localized PECVD process”, Plasma Souces Sci. Tech. 29, 025023 (2020).

Chemical Analysis and Imaging Interfaces Focus Topic
Room 302 - Session CA+2D+AS+BI+HC+LS+NS-TuA

In Situ Microscopy, Spectroscopy and Processing at Liquid-Solid-Gas Interfaces

Moderators: Andrei Kolmakov, National Institute of Standards and Technology (NIST), **Xiao-Ying Yu**, Oak Ridge National Laboratory, USA

2:20pm **CA+2D+AS+BI+HC+LS+NS-TuA-1 Understanding Charge Carrier Variations on the Nanoscale Using Microwave Near-Field Microscopy**, ***T. Mitch Wallis***, *S. Berweger, P. Kabos,* National Institute of Standards and Technology **INVITED**

Understanding the spatial distributions of charge carriers and their polarity in nanoscale semiconductors and their devices remains a long-standing challenge. Scanning probe-based microwave impedance microscopy (MIM, also called scanning microwave microscopy, SMM) can directly probe charge-carriers on the nanoscale via the high-frequency capacitive interaction between the sharp tip and sample of interest.

Here we will first provide an overview of MIM, including applications to model systems. We will then focus on studies of active devices of semiconducting materials, including GaN nanowires and 2D crystals of elemental tellurium. We will conclude with an overview of recent efforts on photoconductivity mapping in 2D materials and hybrid organic-inorganic lead-halide perovskite thin films. In particular, for the latter we leverage the high bandwidth inherent in the microwave signal to obtain temporal resolution as high as 5 ns.

3:00pm **CA+2D+AS+BI+HC+LS+NS-TuA-3 Oxidation/Reduction of Cu Nanoparticles at a Single-Layer Graphene/Electrolyte Interface Monitored by Scanning Kelvin Probe Microscopy**, ***Sidney Cohen***, *S. Khatun, M. Andres, I. Pinkas, I. Kaplan-ashiri, O. Brontvein,* Weizmann Institute of Science, Israel*; I. Rosenhek-Goldian,* weizmann Institute of Science, Israel*; R. Weatherup,* Oxford University, UK*; B. Eren,* Weizmann Institute of Science, Israel

The need to probe chemical and physical processes occurring in at liquid/solid interfaces at small scales is being addressed by several cutting-edge techniques. Scanning probe microscopy (SPM) is now a well-established tool for simultaneous morphological, electrical, and mechanical characterization at the nanoscale. Scanning Kelvin Probe microscopy (SKPM) is an SPM method which can measure the work function at nm distance scales. This technique is not conveniently applied within a solution environment. In this work, micro-electrochemical cells were capped by a single layer graphene upper membrane which is transparent to the electrostatic field, enabling high resolution surface measurements of electrical processes occurring at the interfacial liquid region below the membrane. This talk will present this set-up, and show how it can be used to examine stability, and surface interactions in the oxidation/reduction processes of copper nanoparticles (NPs) attached to the graphene under operating (operando) conditions. Complementary techniques including cyclic voltammetry, and ex-situ electron microscopy and x-ray photoelectron spectroscopy gave a complete description of the processes. As an established catalyst for CO_2 reduction, the behavior of Cu in electrochemical conditions is of great interest in both science and technology. The measurements described here provided a nm-scale view of differences in Cu NP oxidation in ambient air and electrochemical conditions, detecting both a galvanic corrosion in air, and reversible reduction of the NPs at cathodic potentials in alkaline solution. Detachment of the NPs after long measurements of redox cycling is documented and rationalized.

3:20pm **CA+2D+AS+BI+HC+LS+NS-TuA-4 Investigation Tritium and Lithium transport along the Tritium-Producing Burnable Absorber Rod**, ***Jiyoung Son***, Pacific Northwest National Lab*; J. Gao,* PNNL*; G. Sevigny, S. Tripathi, B. Matthews,* Pacific Northwest National Lab*; X. Yu,* Oak Ridge National Laboratory

The compositional and microstructural changes in functional materials are critical for nuclear materials in fusion and fission applications. We investigated tritium (^{3}H) and lithium isotope (^{6}Li, ^{7}Li) transport within a neutron-irradiated target rod, aka, Tritium-Producing Burnable Absorber Rod (TPBAR), used in a light water reactor. TPBARs employ the iron aluminide-coated austenitic stainless-steel cladding and associated cruciform as key components. We used multimodal imaging tools and studied the specimens from irradiated TPBAR components. Specifically, a scanning electron microscope with focused ion beam (SEM-FIB) was used to prepare lift-out samples of the irradiated coating and cruciform samples for follow-up microanalysis. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) was utilized to detect light isotopes in relation to tritium and lithium diffusion and transport. The observed distributions in the irradiated cladding specimens suggest light isotope mobility between internal target components as a result of neutron irradiation. We compared irradiated claddings of two different configurations in SIMS, and the chemical mapping and depth profiles of aluminide coatings show distinct light isotopic distributions. The cruciform specimens extracted from corresponding locations to the claddings also give interesting results. Overall, advanced correlative imaging results confirm tritium diffusion and lithium transport during the tritium production process. Such results give new insights into the fundamental transport mechanism within the target during irradiation and under non-equilibrium, extreme conditions.

4:20pm **CA+2D+AS+BI+HC+LS+NS-TuA-7 Development of a Workflow for Multiscale Elemental Analysis with X-ray Fluorescence Microscopy and Tomography**, ***Si Chen***, Argonne National Lab*; Y. Luo,* Argonne National Laboratory*; T. Paunesku,* Northwestern University*; O. Antipova, Y. Liu, N. Zaluzec, Z. Di,* Argonne National Laboratory*; G. Woloschak,* Northwestern University **INVITED**

Scanning X-ray fluorescence (XRF) microscopy and tomography provides powerful capabilities to assess the elemental distribution in a three-dimensional (3D) space and differentiate their inter- and intra-cellular interactions in complex biological cells and tissues. Like other microscopy techniques, there is often a tradeoff between spatial resolution and field-of-view that each XRF instrument can provide. For example, XRF nanoprobes are specialized for analysis with <50 nm resolution, but the region can be analyzed within a reasonable time frame is limited to only a few tens of microns. Therefore, the capability to combine the use of multiple instruments becomes important for hierarchical analysis.

In this presentation, we will discuss the Bionanoprobe (BNP) instrument and applications. The BNP is an XRF nanoprobe located at the Advanced Photon Source of Argonne National Laboratory. It is dedicated to the studies of biological tissues and cells with a subcellular spatial resolution. In conjunction with a microscale-resolution XRF instrument, we have demonstrated a workflow to perform multiscale elemental mapping and tomography on HeLa cells treated with non-targeted nanoparticles. While nanoscale tomography revealed the nanoparticle distribution in individual cells, statistical information on cell-nanoparticle interaction was obtained with the microprobe from a large population of cells.

It is important to note the challenges in sample preparation for such multiscale analysis across platforms. Different instruments often require different specimen dimensions in order to achieve their optimal performance. To enable analysis on the same specimen, we have introduced an intermediate specimen manipulation step between micro- and nano-scale measurements utilizing focused ion beam (FIB). Local regions of interest identified with the microprobe were isolated with a FIB instrument and further analyzed at the BNP. Angular enlargement for tomography data collection enabled by the FIB operation significantly improved the tomography reconstruction quality.

5:00pm **CA+2D+AS+BI+HC+LS+NS-TuA-9 in Situ Molecular Imaging of Green Solvents for CO_2 Capture**, ***Xiao-Ying Yu***, Oak Ridge National Laboratory, USA

Switchable ionic liquids are emerging green solvents in for carbon dioxide (CO_2) capture, cleaner separation, and efficient biomass production.However, the liquid structure and composition of SWILs are not fully understood.Besides off-line analyses using NMR and IR, our knowledge of the sustainable green solvents is limited.We used in situ liquid time-of-flight secondary ion mass spectrometry (ToF-SIMS) to study such solvents in this work.This is a unique in situ molecular imaging technique enabled by the invention of a vacuum compatible microfluidic reactor termed system for analysis at the liquid vacuum interface (SALVI).Green solvents of interest were synthesized and reported previously. They were introduced into the microfluidic channel for in situ analysis using liquid ToF-SIMS.Two model systems are illustrated in this talk.The first consists of 1, 8-diazabicycloundec-7-ene (DBU) and 1-hexanol with different CO_2 loadings.The second has koechanol with various CO_2 loadings.Koechanol acts as both acid and base in the latter.Our results show two coexisting liquid phases in these green solvents.This phenomenon was only hypothesized in previous theory prediction.We provide the first physical evidence of the complex liquid – liquid (l – l) interface using three-dimensional chemical mapping with submicrometer

resolution.In addition, more complex stoichiometry is discovered due to CO_2 uptake.More importantly, we have provided the first chemical spatial visualization elucidating the evolving l – l interface.The more detailed molecular level understanding of the liquid structure and composition are instrumental to build the foundation for predicative material synthesis, CO_2 capture, and other versatile applications.

5:20pm **CA+2D+AS+BI+HC+LS+NS-TuA-10 Depth Dependence of Salt Ions at the Liquid/Vapor Interface Studied by Ambient Pressure X-Ray Photoelectron Spectroscopy**, *A. Siebert, K. Goodman,* ***Monika Blum***, LBNL

Liquid/vapor interfaces play an important role in chemical, biological, technological, and environmental processes. Perhaps one of the most important interfaces for the environment is the interface between atmospheric aqueous aerosols and the surrounding air, which affects reactions like the scattering and absorption of sunlight as well as the probability of aerosols to serve as cloud condensation nuclei. [1,2] However, the experimental investigation of this active region is complicated by the necessary pressures far away from the ultra-high-vacuum (UHV) region, which is usually required in most surface science studies.[3]

In the recent past, ambient pressure X-ray photoelectron spectroscopy (APXPS) has proven to be a very powerful tool to study the chemical and electronic structure of liquids, solutions, and their interfaces with different media, not requiring the UHV conditions of standard XPS measurements. In this contribution we will utilize a colliding micro flat jet system with synchrotron-based APXPS to gain full insight into the depth dependency of different aqueous salt solutions, e.g. $CaCl_2$,at low salt concentrations. We will present a comparison of bulk ion concentrations in aqueous salt solutions and the surface ion concentration obtained from the ratio between the probed core level area and the peak area of the liquid water phase. This allows us to model the depth profile of salt ions in aqueous solutions and to correlate the data with existing theoretical models.

[1] Havala O. T. Pye et al., Atmos. Chem. Phys., 20, 4809–4888, 2020. [2] Barbara J. Finlayson-Pitts, Phys. Chem. Chem. Phys., 2009, 11, 7760–7779.

Nanoscale Science and Technology Division
Room Ballroom A - Session NS-TuP

Nanoscale Science and Technology Poster Session

NS-TuP-1 Collection of Raman Signal in a Liquid Using Plasmonic Vortex Fiber, ***Rohil Kayastha***, *B. Birmingham, Z. Zhang,* Baylor University

Tip-enhanced Raman spectroscopy (TERS) has been demonstrated to achieve nanoscale resolution by focusing the light beam at the tip directly from the free space using the surface plasmon polariton (SPP). Conventional TERS applications possess problems such as low excitation and collection efficiency, optical alignments, and so on. Application of TERS in a liquid environment exposes additional challenges because of difficulty in focusing the excitation beam as the beam diffracts at the air-liquid interface between different refractive indexes. Here, a plasmonic fiber-based TERS, using SPP in a conical Kretschmann configuration, nano-focuses the radially polarized beam at the tip apex to excite and uses the back-collection method to collect the Raman signals to overcome the aforementioned challenges.

A tapered fiber was gold (Au) coated to be used as the plasmonic tip for TERS. Both linear and radial polarized beams can plasmonically excite into SPP mode at the tapered region, however, only a radial polarized mode can be localized without destructively interfering which achieves nano-focused light at the tip apex. Therefore, vortex fiber, a polarization-maintaining optical fiber, was used to guide the radially polarized mode. The plasmonic excitation of vortex fiber with internal illumination of the radially polarized beam was studied to demonstrate nano-focusing of the light beam near the tip apex using a liquid sample. The concentration dependence of the plasmonic coupling in the liquid sample was demonstrated. The Raman signal displayed dependence on the refractive index of the liquid as the concentration of the solution changed. Stronger Raman signals at the air-liquid interface were observed in comparison to when the fiber tip was fully submerged into the liquid which is due to the combination of the coupling of the waveguided mode from the fiber to the SPP mode and to a waveguided mode in the tapered liquid layer that forms over the tip. The air-liquid interface experiment also demonstrates that most of the signal is obtained near the tip apex than from the shaft of the probe. The plasmonic tip has been incorporated into a near field scanning optical microscope (NSOM) to obtain the topographical and spectroscopic information on a substrate with nanoscale resolution. The polarization dependence of the light beam (radial and azimuthal polarization) will also be tested to compare and understand the plasmonic coupling to enhance the coupling efficiency thus, enhancing the Raman signal.

NS-TuP-2 Chemical Mechanical Planarization Slurry Stability Study, ***Yibin Zhang***, FUJIFILM Electronic Materials USA., Inc.

The stability of slurry for Chemical Mechanical Planarization (CMP) is one of the big concerns in semiconductor fabs. It might potentially be a deal-killer for its application due to its short period of stability even though it has a good performance in other aspects, like removal rate, erosion, and dishing. one of the main reasons for defectivity, an important factor of slurry performance in the CMP process, is the presence of large agglomerates in the slurry. As a result, lots of efforts have been done to stabilize of slurry and formulate highly stable slurries, which minimize the formation of oversize agglomerates. A highly stable CMP slurry is critical to reduce process-dependent defectivity such as scratches and particle residues.

In this work, we present a novel optical technique, MultiScan Emulsion and Dispersion Stability Analyzer, which can efficiently and accurately check the stability of certain formulations of the slurries or screen raw materials and their combination's stability. A few samples will be analyzed to demonstrate the capability of stability investigation by using this technique. In the meantime, the traditional stability test method will be used as well for comparison. We propose some mechanisms respectively for stability for each sample. This technique will save >50% time for routine shelf-life stability study compared to the traditional test method.

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NS-TuP-3 A New Tool for Quantum and Nanoscale Materials Engineering, ***Gianfranco Aresta***, Ionoptika Ltd, UK

Quantum computing is the next great frontier of science. It has the potential to revolutionise many aspects of modern technology, including digital communications, "quantum-safe" cryptography, as well as incredibly accurate time measurements.

Single impurity atoms in semiconductors are receiving attention as potential quantum technologies, and proof-of-concept devices have shown promise. However, such devices are incredibly challenging to manufacture, as single atoms must be placed within ~ 20 nm of each other within a pure ^{28}Si matrix.

All working devices thus far have been fabricated using hydrogen lithography with an STM followed by atomic layer deposition. It is labour-intensive and requires several days of meticulous preparation to create just a single quantum bit (qubit). Real-world devices will require arrays of hundreds or thousands of impurity atoms, highlighting the requirement for a scalable method of positioning single atoms with nanometre precision.

We report on a new commercial instrument for the fabrication of quantum materials and devices via ion implantation. A well-established technique in the semiconductor industry, ion implantation is both flexible and highly scalable. The instrument features a high-resolution mass-filtered focused ion beam (FIB), a high-sensitivity deterministic implantation system, 6-inch wafer handling, and a high-precision stage.

The ion dose delivered to the sample can be adjusted across a wide range, providing several materials engineering capabilities in a single tool. The deterministic implantation system allows single ion implantation with confidence levels as high as 98%. Operating in a high beam current mode provides direct-write capabilities such as isotopic enrichment and targeted ion-implantation of nanomaterials such as nanowires and graphene.

The liquid metal ion source and mass filtered column can implant many different elements with isotopic resolution. Available sources include silicon, erbium, gold, and bismuth, while many others of technological interest are in development.

NS-TuP-4 Atomic Silicon Wires: Dopant Mediated Charging Characterization, ***Max Yuan***, University of Alberta, Canada; *R. Wolkow,* University of Alberta, Quantum silicon, Canada; *R. Achal, J. Croshaw,* Quantum Silicon, Canada; *T. Chutora, F. Altincicek, C. Leon,* University of Alberta, Canada; *L. Livadaru,* Quantum silicon, Romania; *J. Pitters,* Quantum silicon, Canada

CMOS technologies are approaching their performance limits. Atomic silicon electronics are poised to provide the next-generation of devices. This beyond CMOS platform consists of exactingly patterned dangling bond (DB) circuitry on hydrogen passivated silicon (H-Si).[1] Many passive and active components can be made of DBs, here we investigate atomic silicon wires. We employ a recent dopant based charge sensing procedure in conjunction with non-contact atomic force microscopy to study the charging behavior of atomically fabricated DB wires on H-Si (100) 2x1. On its own, this method can be used to rapidly detect local net charge with single electron sensitivity; coupled with AFM, it can drastically improve confidence in data interpretation.[2] In this scheme, a single DB sensor is employed to detect a sharp step in its I(V) spectroscopy due to the ionization of a nearby arsenic dopant. As charged DBs are fabricated nearby, local band bending shifts the dopant ionization voltage which can act as a charge sensor. Wires, both parallel and perpendicular to the dimer direction were systematically lengthened and studied using this method. The charging behavior for various lengths of wire, and novel observations, such as a length dependent flip flop in electron occupation for perpendicular wires are demonstrated. This method and these results will be used to improve the characterization of DB structures and will eventually be directly compared to theory to improve the modeling of DB circuitry.

Huff, T., Labidi, H., Rashidi, M., Livadaru, L., Dienel, T., Achal, R., Vine, W., Pitters, J., & Wolkow, R. A. (2018). Binary atomic silicon logic. Nature Electronics, 1(12), 636–643. https://doi.org/10.1038/s41928-018-0180-3

Achal, R., Rashidi, M., Croshaw, J., Huff, T. R., & Wolkow, R. A. (2020). Detecting and Directing Single Molecule Binding Events on H-Si(100) with Application to Ultradense Data Storage. ACS Nano, 14(3), 2947–2955. https://doi.org/10.1021/acsnano.9b07637

2D Materials Technical Group
Room 303 - Session 2D+EM+MI+NS+QS-WeM

2D Materials: Quantum and Symmetry-Protected States

Moderators: Thomas Michely, University of Cologne, Germany, **Frances Ross**, Massachusetts Institute of Technology

8:00am **2D+EM+MI+NS+QS-WeM-1 Semi-High Throughput Investigation of 2d Materials: Anomalous Quantum Confinement Effect and Spectral Properties**, ***Francesca Tavazza***, *K. Choudhary,* National Institute of Standard and Technology **INVITED**

Materials with van der Waals-bonding exhibit quantum confinement effect, in which the electronic bandgap of the three-dimensional (3D) form is lower than that of its two-dimensional (2D) counterpart. However, the possibility of an anomalous quantum confinement effect (AQCE) exists, where the bandgap trend is reversed. In this work, we computationally identify materials with AQCE. Using density functional theory (DFT), we compute ≈1000 OptB88vdW (semi-local functional), ≈50 HSE06 and ≈50 PBE0 (hybrid functional) bandgaps for bulk and their corresponding monolayers, in the JARVIS-DFT database. OptB88vdW identifies 65 AQCE materials, but the hybrid functionals only confirm such finding in 14 cases. Electronic structure analysis shows that AQCE is often characterized by the lowering of the conduction band in the monolayer and related changes in the p_z electronic orbital contribution. In addition to AQCE, the JARVIS-DFT contains IR and Raman spectra for many 2D materials. Properties of such spectra will be discussed as well.

8:40am **2D+EM+MI+NS+QS-WeM-3 Dry Patterning Chemically Sensitive Quantum Materials**, ***Joseph Benigno***, *Q. Zou, C. Cen, L. Li,* West Virginia University

Accurate, repeatable patterning of quantum material-based electronic devices is desirable for electrical transport measurements. However, the most common method, photolithography, can degrade, or even damage, chemically sensitive quantum materials during fabrication. Here we introduce a new dry-patterning method for device fabrication with lateral etching resolution down to ~30 µm. The new method utilizes a tabletop computer numerical control (CNC) router machine to gently etch patterns into thin films, leaving behind the desired device or devices on the substrate. We create Hall bars with conductive channel widths of 30, 60, and 120 µm from ~20 layer FeTe-capped superconducting single layer FeSe/$SrTiO_3$ systems. Transport measurements show the same zero resistance T_c of 10 K for the Van der Pauw (vdP) geometry and all Hall bar structures. However, the onset temperature T_{onset} is the largest at 28K for the vdP geometry, and decreases with the width of the Hall bar to 13K for the 60 µm device. Our method provides a new time-saving, cost-effective, and chemical-free strategy for fabrication of devices from quantum materials.

This research is supported by DOE DE-SC0021393.

9:00am **2D+EM+MI+NS+QS-WeM-4 Electron Transport and Charge Sensing in Strongly Coupled Quantum Dot Array in Silicon**, ***Fan Fei***, *J. Wyrick, P. Namboodiri, J. Fox,* NIST*; E. Khatami,* SJSU*; R. Silver,* NIST

Atomically precise donor-based quantum devices in silicon are fabricated using STM lithography, which has become a promising platform for solid state quantum computation and analog quantum simulation. Lattices of dopant-based quantum dots have unique advantages in simulating strongly correlated Fermionic systems of real atomic lattice sites because of their naturally occurring ion-cores which make them the Fermi-Hubbard sites in the Silicon Vacuum. Understanding electron transport and charge configuration in a smaller array is critical to using these arrays to simulate larger systems and explore various condensed matter physics phenomena such as superconductivity in the future. This talk will focus on the electron transport in the strongly coupled regime where the electrons delocalize across small N x N dot arrays. Numerical simulations for charge stability diagrams and transport properties show qualitatively agreement with our experiments. We apply rf reflectometry on a SLQD and use it as charge sensor for probing the electron configuration within the array.

9:20am **2D+EM+MI+NS+QS-WeM-5 Observation of the Layer Hall Effect in Topological Axion Antiferromagnet $MnBi_2Te_4$**, ***Suyang Xu***, Harvard University **INVITED**

While ferromagnets have been known and exploited for millennia, antiferromagnets were only discovered in the 1930s. The elusive nature indicates antiferromagnets' unique properties: At large scale, due to the absence of global magnetization, antiferromagnets may appear to behave like any non-magnetic material; At the microscopic level, however, the opposite alignment of spins forms a rich internal structure. In topological antiferromagnets, such an internal structure leads to a new possibility, where topology and Berry phase can acquire distinct spatial textures. We study this exciting possibility in an antiferromagnetic Axion insulator, even-layered $MnBi_2Te_4$ flakes. We report the observation of a new type of Hall effect, the layer Hall effect,where electrons from the top and bottom layers spontaneously deflect in opposite directions.

Reference:

A. Gao, et al."Layer Hall effect in a 2D topological axion antiferromagnet." *Nature* 595, 521 (2021).

11:00am **2D+EM+MI+NS+QS-WeM-10 Phonon Limited Mobility and Phonon Drag in h-BN Encapsulated Monolayer and AB-stacked Bilayer Graphene**, ***Vasili Perebeinos***, University at Buffalo

We report the electrical transport in h-BN encapsulated AB-stacked bilayer graphene theoretically and experimentally. Using the perturbation theory within the tight-binding model approach, we identify the dominant role of the shear phonon mode scattering on the carrier mobility in AB-stacked graphene bilayer at room temperature. The shear phonon mode is absent in free-standing monolayer graphene, which explains high mobilities in monolayer devices fabricated under similar conditions resulting in minimal Coulomb impurity scattering. At temperatures above 200K, the surface polar phonon scattering from the boron-nitride substrate contributes significantly to the experimental mobilities of 15,000 -20,000 cm^2/Vs at room temperature and carrier concentration n~10^{12} cm^2 reported here. A screened SPP potential for a dual gated bilayer and transferable tight-binding model allows us to predict mobility scaling with temperature and bandgap for both electrons and holes in agreement with the experiment Phys Rev. Lett. 128, 206602 (2022).

The resulting electron-SPP coupling is used to predict that, by exploiting the strong coupling of their electrons to surface polar phonons, van der Waals heterostructures can offer a suitable platform for phonon sensing, capable of resolving energy transfer at the single-phonon level. The geometry we consider is one in which a drag momentum is exerted on electrons in a graphene layer, by a single out-of-equilibrium phonon in a dielectric layer of hexagonal boron nitride, giving rise to a measurable induced voltage. Our numerical solution of the Boltzmann Transport Equation shows that this drag voltage can reach a level of a few hundred microvolts per phonon, well above experimental detection limits. Furthermore, we predict that drag voltage should be largely insensitive to the mobility of carriers in the graphene layer and increase the temperature up to at least 300 K, offering the potential of a versatile material platform for single-phonon sensing.

11:20am **2D+EM+MI+NS+QS-WeM-11 Exciton Physics at the Atomic Scale**, ***Daniel Gunlycke***, U.S. Naval Research Laboratory

Descriptions of excitons in pristine semiconducting crystals usually rely on the hydrogen model adopted for excitons. Owing to the weak screening in monolayer transition-metal dichalcogenides, however, the electron and hole separation in the strongest bound excitons is on the atomic scale, necessitating atomistic treatment. In this presentation, we present a minimalistic exciton model that accounts for the lattice and the spin-orbit and exchange interactions, thus making this model appropriate across the spectrum from Wannier to Frenkel excitons. Using this model, we show that the exciton lifetimes could be extended by transitioning the excitons into excitonic dark states. Longer exciton lifetimes could make these materials candidates for applications in energy management and quantum information processing.

11:40am **2D+EM+MI+NS+QS-WeM-12 Weyl Semimetals with Low-Symmetry Crystal Structure for Generating Out-of-Plane Oriented Spin Current**, ***Simranjeet Singh***, Carnegie Mellon University **INVITED**

Weyl semimetals (WSMs), such as WTe_2 and $MoTe_2$, host plethora of novel phenomena that are highly relevant for quantum spintronics, namely: Dirac type dispersion, strong spin-orbit coupling (SOC), Fermi arcs, and helical spin-momentum locked surface and bulk states. WSMsprovide a distinct opportunity to obtain highly efficient and unconventional charge to spin conversion owing to strong SOC, symmetry breaking, and these topology-based phenomena. On the other hand, spin-orbit torque (SOT) driven deterministic control of the magnetic state of a ferromagnet with perpendicular magnetic anisotropy is key to next generation spintronic applications including non-volatile, ultrafast, and energy efficient data

storage devices. But field-free deterministic SOT switching of perpendicular magnetization remains a challenge because it requires an out-of-plane oriented spin current, which is not allowed in conventional spin source materials such as heavy metals and topological insulators due to the system's symmetry. The exploitation of low-crystal symmetries WTe_2 and $MoTe_2$ offers a unique approach to achieve SOTs with unconventional forms[1]. In this work, I will discuss our experiments to realize field-free deterministic magnetic switching of a perpendicularly polarized van der Waals magnet employing an out-of-plane spin current generated in layered WTe_2, which is a quantum material with low-symmetry crystal structure[2]. I will also discuss our experiments aimed at achieving field-free SOT switching of semiconducting and insulating FMs using spin current in WSMs. Our work establishes transition metal dichalcogenides, with lower symmetry crystal structure, as an appealing spin source material for future spin-orbit torque related magnetic memory technologies.

[1]. MacNeill, D. *et al.* Control of spin–orbit torques through crystal symmetry in WTe_2/ferromagnet bilayers. *Nature Physics***13**, 300-305, (2017).

[2]. Kao, I-H *et al.* Deterministic switching of a perpendicularly polarized magnet using unconventional spin–orbit torques in WTe_2. Nature Materials (2022). https://doi.org/10.1038/s41563-022-01275-5

Nanoscale Science and Technology Division
Room 304 - Session NS+AP+BI+SS-WeM

Frontiers in Scanning Probe Microscopy Including Machine Learning

Moderators: Wonhee Ko, University of Tennessee, Knoxville, **Adina Luican-Mayer**, University of Ottawa, Canada

8:40am **NS+AP+BI+SS-WeM-3 Decay Rate Spectroscopy for a Direct Probe of Josephson and Andreev Currents on the Atomic Scale***, **Wonhee Ko,*** University of Tennessee, Knoxville*; J. Lado,* Aalto University, Finland*; E. Dumitrescu, P. Maksymovych,* Oak Ridge National Laboratory

The tunneling current in superconducting tunnel junctions involves several mechanisms in addition to the normal-electron tunneling, such as Josephson tunneling and Andreev reflection. Identification of the tunneling mechanisms as a function of external parameters, such as barrier height, bias voltage, temperature, and so on, is the key to elucidating the characteristics of the superconductors, such as paring symmetry and topology. Here, we present a method to identify distinct tunneling modes based on the decay rate of tunneling current measured by scanning tunneling microscopy (STM) [1,2]. Precise control of the tip-sample distance in picometer resolution allows us to quantify the decay rate as a function of bias *V* and tip height *z*, with which we identified the crossover of tunneling modes between single-charge quasiparticle tunneling, (multiple) Andreev reflection, and Josephson tunneling. The method was both applied to S-I-S [1] and S-I-N [2] junctions, to unambiguously identify Josephson and Andreev currents. Moreover, mapping decay rates in the atomic resolution with STM revealed the intrinsic modulation of Andreev reflection and Josephson current. The result shows that the decay rate spectroscopy will be crucial for addressing the superconducting characteristics of the materials and their applicability for Josephson-junction devices.

This research was performed at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility.

[1] W. Ko, E. Dumitrescu, and P. Maksymovych, *Phys. Rev. Res.***3** 033248 (2021)

[2] W. Ko, J. L. Lado, and P. Maksymovych, *Nano Lett.***22** 4042 (2022)

9:00am **NS+AP+BI+SS-WeM-4 Machine Learning-Driven Automated Scanning Probe Microscopy: Application to Ferroelectric Materials***, **Yongtao Liu**, K. Kelley, R. Vasudevan,* Oak Ridge National Laboratory, USA*; H. Funakubo,* Tokyo Institute of Technology, Japan*; S. Kalinin,* University of Tennessee Knoxville*; M. Ziatdinov,* Oak Ridge National Laboratory, USA

Scanning probe microscopy (SPM) has become a mainstay of many scientific fields including materials science, condensed matter physics, and so on. Machine learning (ML) and artificial intelligence (AI) have been applied to determine the physical mechanisms involved in phenomena encoded within microscopy data, enabling ML/AI to rapidly become an indispensable part of physics research. However, the real-time connection between ML and microscopy—which enables automated and autonomous experiments for microscopy imaging and spectroscopy measurements—still lags. Until now, the search for interesting functionalities in microscopy experiments has been guided by auxiliary information from microscopy to identify potential objects of interest based on human intuition; the exploration and verification of physical mechanisms depend on human-based decision making, i.e., operators determine the parameters for subsequent experiments according to the previous experiment. Here, we developed ML-driven automated experiment (AE) scanning probe microscopy (SPM) workflow to learn the functionality and mechanism in materials in an automatic manner. We demonstrate the application of deep kernel learning and hypothesis learning based workflows by investigating ferroelectric materials, including studies of domain wall dynamics, domain switching mechanism, the conductivity of topological defects, and relationship between domain structure and local properties. Using these approaches, we observe larger hysteresis opening near 180° domain walls due to the larger polarization mobility in the vicinity of the 180° walls in a $PbTiO_3$ sample and find that the domain switching in a $BaTiO_3$ thin film is determined by the kinetics of the domain wall motion, etc. We implemented these approaches in SPM for ferroelectric materials investigation, however, the workflows are universal and can apply to a broad range of imaging and spectroscopy methods, e.g., electron microscopy, optical microscopy, and chemical imaging.

Acknowledgements: This work (implementation, measurement, and data analysis) was primarily supported by the center for 3D Ferroelectric Microelectronics (3DFeM), an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences under Award Number DE-SC0021118. This work (ML development) was supported by the Center for Nanophase Materials Sciences, a US Department of Energy Office of Science User Facility.

9:20am **NS+AP+BI+SS-WeM-5 AVS Dorothy M. and Earl S. Hoffman Scholarship Talk: Direct Imaging of Light-Matter Interaction of 0-dimensional Excitonic Emitters using Tip-enhanced Scanning Probe Technique***, **Kiyoung Jo***[1]*, E. Marino, J. Lynch, Z. Jiang, N. Gogotsi,* University of Pennsylvania*; P. Schuck,* Columbia University*; N. Borys,* Montana State University*; C. Murray, D. Jariwala,* University of Pennsylvania

Strong light-matter interactions of 0-dimensional emitters on plasmonic Au substrate were explored using both contact and tapping mode tip-enhanced scanning probe micro-spectroscopy. The plasmonic tip engaged with contact mode couples with the excitonic dipole in CdSe-CdS nanoplatelets, leading to strong exciton-plasmon coupling. Unlike the contact mode, the directional propagation of surface plasmon polariton from the excitonic emission of the nanoplatelets on Au as wave-like fringe patterns was probed by taking advantage of the tapping mode. Since tapping mode operates a few nanometers away from the surface, the near-field photoluminescence with in-plane wavevectors can be collected, leading to form fringe patterns propagating from the quantum plate. Extensive optical simulations proved that the fringes are the result of standing wave formed between the tip and the nanoplatelets. The effect of excitonic dipole orientation and dielectric layers on the fringe patterns were investigated by the simulation which matched with experimental results. The fringe patterns were also observed in WSe2 nano-bubbles, and the CdSe/CdS nanoplatelet in SiO2/Si substrate which means the phenomenon is universal in 0-dimensional emitters and various substrates. We envision that the discovery excels in understanding in-plane near-field light signal transduction from 0-dimensional emitters toward nano and quantum photonics.

9:40am **NS+AP+BI+SS-WeM-6 Nanoscale Subsurface Depth Sensitivity of Contact Resonance Atomic Force Microscopy on Layered Films***, **Gheorghe Stan,*** National Institute for Science and Technology (NIST)*; C. Ciobanu,* Colorado School of Mines*; S. King,* Intel Corporation

Probing the mechanical properties is one of the basic inquiries that can reveal the structure and integrity of an isolated material or multicomponent system. At the nanoscale, due to size constrains and defects, mechanical tests become even more relevant as the properties of a part may differ by those of the whole. Over years, contact resonance AFM (CR-AFM) has proved to be a reliable AFM-based technique for nanoscale mechanical property measurements. Mostly operated into the elastic modulus range from few GPa to hundreds of GPa, CR-AFM was used to test different materials and structures at the nanoscale and considered for discerning the mechanical response of subsurface inhomogeneities and buried domains. It remains, however, to directly prove the extent of its quantitative capabilities both in terms of elastic modulus and depth

[1] **AVS Dorothy M. and Earl S. Hoffman Scholarship Recipient**

sensitivity. In this work, we develop a quantitative methodology to test the elastic modulus and depth sensitivity of CR-AFM against a set of low-k dielectric bilayer films with the top layer of various thicknesses. We have analyzed the measured contact stiffness as a function of load and film thickness with both a semi-analytical model and three-dimensional finite element analysis. Both analyses confirmed the expected elastic moduli of the layered structures and provided a robust quantitative estimation of the subsurface depth and material sensitivities of CR-AFM. We also developed a correlative measurement-model analysis to assess the convoluted contributions of the structural morphology and mechanical properties to the contact stiffness used by AFM-based subsurface imaging. The results explain the inherent difficulties associated with solving concurrently the material contrast and location of subsurface heterogeneities in nanomechanical subsurface imaging.

11:00am **NS+AP+BI+SS-WeM-10 The Impact of Temperature on Viscoelastic Properties of Nanoscale Domains Within Polymer Composites**, ***Bede Pittenger***, *S. Osechinskiy, J. Thornton, S. Loire, T. Mueller,* Bruker Nano Surfaces

The behavior of polymer composites is controlled by the properties of the components as well as the microstructure of the material. Because confinement effects and interphase formation can alter properties of the microphases, only measurements performed directly on the composite can provide the needed local property distribution. Mechanical properties of polymers are generally temperature (and time) dependent, so a full understanding requires measurements over a range of temperatures and frequencies. Ideally, one would like to observe the mechanical behavior of these microscopic domains while they pass through their glass transitions to appreciate the influence of size effects and confinement on time dependent mechanical properties.

Recently, Atomic Force Microscopy based nano-Dynamic Mechanical Analysis (AFM-nDMA) was introduced. Like bulk DMA, this mode provides spectra of storage and loss modulus across frequency and temperature, allowing construction of master curves through Time Temperature Superposition (TTS). In addition, it allows high resolution measurements localized to the microscopic structures within heterogeneous samples. This presentation will examine the capabilities of this new mode with examples in a wide range of polymers and composites.

11:20am **NS+AP+BI+SS-WeM-11 AFM Force Spectroscopy Combined with Machine-Learning Methods for Identifying Malaria Derived- EV Subpopulations**, ***Irit Rosenhek-Goldian***, *P. Abou Karam,* Weizmann Institute of Science, Israel*; T. Ziv,* Technion - Israel Institute of Technology, Israel*; H. Ben Ami Pilo, I. Azuri, A. Rivkin, E. Kiper, R. Rotkopf, S. Cohen,* Weizmann Institute of Science, Israel*; A. Torrecilhas,* Federal University of São Paulo, Brazil*; O. Avinoam,* Weizmann Institute of Science, Israel*; A. Rojas,* University of Costa Rica*; M. Morandi, N. Regev-Rudzki,* Weizmann Institute of Science, Israel

The Malaria (*Plasmodium falciparum*) parasite releases extracellular vesicles (EVs) which modulate the mechanical properties of the host red blood celland thus facilitate parasite action. It is understood that EVs are composed of sub-populations with different functions, but little is known of their nature and specialized function. Here, we report the use of Atomic Force Microscopy (AFM) imaging and puncture analysis, combined with state-of-the-art size separation techniques and several biochemical, microscopic and spectroscopic characterization techniques in an attempt to differentiate and characterize the different populations. Specifically, we subjected malaria-derived EVs to size-separation analysis, using Asymmetric Flow Field-Flow Fractionation (AF4). The fractions obtained were characterized by Cryo-transmission electron microscopy (cryo-TEM), and AFM which revealed the presence of two distinct EV subpopulations - small (10-70 nm) and large (30-500 nm). Proteomic analysis revealed that the small EVs were enriched in complement-system proteins and the large EVs with proteasome subunits. In addition, Förster resonance energy transfer (FRET)-based fusion assay showed that small EVs fused to early-endosome liposomes at significantly greater levels than large EVs. Finally, AFM puncture analysis characterized by unsupervised machine-learning verified the presence of two distinct fractions with respect to mechanical behavior which correlate with the EV size groupings. These results shed light on the sophisticated mechanism by which malaria parasites utilize EV subpopulations as a communication tool to target different cellular destinations or host systems.

Nanoscale Science and Technology Division
Room 304 - Session NS1+BI-WeA

Nanopore Sensing and Fabrication, Operation and Metrology of Biodevices

Moderators: David Czaplewski, Argonne National Laboratory, **Georg Fantner**, EPFL, Switzerland

2:20pm **NS1+BI-WeA-1 Single Cell and Single Molecule Biophysics with Glass Nanopores**, ***Georg Fantner***, *A. Radenovic, S. Leitao, V. Navikas, B. Drake,* EPFL, Switzerland **INVITED**

Scanning ion conductance microscopy (SICM) has been around for decades, yet it has not received as much attention as other forms of scanning probe microscopy. Recently, this true non-contact techniquehas kindled renewed interest among biophysicists and biologists because it is ideally suited for label-free imaging of fragile cell surfaces where it achieves exquisite resolution down to the nanometer regime without distorting the cell membrane. SICM uses a glass nanopipette as a scanning probe and measures the current through the glass nanopore as a proximity detection of the sample surface. The challenge to harness this technique for time resolved 3D nanocharacterization of living cells lies in the relatively slow imaging speed of SICM. In this presentation I will show how we apply what we have learned from high-speed AFM to the field of SICM. By reengineering the SICM microscope from the ground up, we were able to reduce the image acquisition time for SICM images from tens of minutes down to 0.5s while extending the imaging duration to days.

SICM, however, is much more versatile than just an imaging tool. I will also discuss our recent results using SICM as a single molecule characterization tool. We term this method scanning ion conductance spectroscopy (SICS). Using capillaries with exceptionally small nanopores, we are able to detect and manipulate single molecules in a repeatable and high throughout manner.

3:00pm **NS1+BI-WeA-3 Ultrasensitive Nanoporous Gold Substrates for SERS Detection in Liquids or Gases**, ***Issraa Shahine***, *B. Humbert, J. Mevellec, M. Richard-Plouet, P. Tessier,* Nantes Université, CNRS, Institut des Matériaux de Nantes Jean Rouxel (IMN), France

The design of three-dimensionally structured, gold nanoporous membranes is described. Our aim is to design surface enhanced Raman scattering (SERS) substrates to detect very low concentrations of molecules in liquid or gaseous phases. The SERS substrates are constituted of stacked ultrathin nanoporous gold thin layers. They are obtained in a two-step process: first deposition of alternative copper and gold stacked nanolayers by magnetron sputtering, and second, chemical etching to dissolve copper, resulting in the nanoporous morphology. The obtained thin layers of gold give rise to superior surface enhanced Raman scattering (SERS) capability using 2,2-bipyridine (BP) as probe molecules for detection. The SERS intensity mapping confirm the presence of hot spots with a low detection limit down to 10^{-18} mol.L^{-1} of BP concentration. The ultrasensitivity at low concentration molecules is assigned to the effects of the localized enhanced electromagnetic fields around the nano ligaments. An additional Raman mechanism is also highlighted by μ-Surface Enhancement Spatially Offset Raman spectroscopy (μ-SESORS): gold ligaments inside nanoporous layers act as waveguides for the incident light, leading to a significant increase in the size of the active SERS area. These SERS substrates have the ability to detect low BP vapor pressure in air.

This process is a reliable method for fabricating uniform, highly reproducible and efficient SERS substrates, with a robust SERS response at extremely low detection limits.

Nanoscale Science and Technology Division
Room 304 - Session NS2+AS+EM-WeA

Scanning Probe Metrology of 1D and 2D Materials

Moderators: Maryam Ebrahimi, lakehead University, Canada, **Aubrey Hanbicki**, Laboratory for Physical Sciences

4:20pm **NS2+AS+EM-WeA-7 New on-Surface Synthesis Techniques for Creating Precise 1D Graphene Nanoribbon Heterojunctions and Device-Tunable 2D Molecular Arrays**, ***Michael Crommie***, UC Berkeley Department of Physics*; G. Dong,* University of Chicago Department of Chemistry*; J. Lischner,* Imperial College London Department of Materials, UK*; A. Zettl, P. Jacobse, Z. Wang,* UC Berkeley Department of Physics*; J. Yin,* University of Chicago Department of Chemistry*; H. Tsai, F. Liou, A. Aikawa,* UC Berkeley Department of Physics **INVITED**

Bottom-up fabrication techniques for assembling molecular nanostructures at surfaces typically exploit various surface interactions that (along with random thermal processes) can be biased toward achieving desired structural results via the clever design of molecular precursors. Great progress has been made using this approach, but surface-grown molecular structures remain plagued by random, uncontrolled processes that make complex structural control difficult. Overcoming this problem is one of the grand challenges of this subfield. Here I will discuss two new approaches to molecular surface assembly that have allowed us to improve order in surface-based nanostructures. The first involves 1D materials and utilizes a solution-based polymerization scheme combined with a new surface deposition procedure. The second involves combining molecular surface assembly with 2D field-effect transistors (FETs). The first method is focused on graphene nanoribbons (GNRs), nanometer-wide strips of graphene. Fabricating complex heterostructure sequences in GNRs remains a difficult challenge because we can't sequence GNRs the way we sequence DNA. This makes it hard to fulfill the promise of GNR-based molecular electronics because of the difficulty of fabricating GNRs composed of well-ordered segments that each have controlled properties (e.g., bandgap, doping, magnetism, optical response). We have made progress toward overcoming this challenge by using a new protecting-group-aided-iterative-synthesis strategy. This allows us to create GNR oligomers with perfectly defined monomer sequences in solution that can be deposited onto surfaces for cyclodehydrogenation using a matrix-assisted deposition (MAD) procedure. This has enabled the synthesis of GNR heterojunctions that would not be possible via other techniques. The second technique I will discuss involves the use of an "active substrate" (a graphene FET) to induce *reversible* 2D molecular assembly through a combination of Coulomb and van der Waals interactions. The trick here is to use a molecule (in our case F_4TCNQ) whose LUMO level (E_L) lies in an energy range accessible to the Fermi level (E_F) of the 2D FET. Manipulating E_F relative to E_L via the device backgate allows charge in the device to reversibly flow between substrate states and the LUMO level of adsorbed molecules. This results in unexpected mechanical responsivity of the molecules, including tunable 2D array formation and a reversible quasi-1D phase transition that we have imaged using scanning tunneling microscopy.

5:00pm **NS2+AS+EM-WeA-9 Temperature-Mediated Adsorption and Assembly of Internally Fluorinated Chevron Graphene Nanoribbon Precursors on Au(111)**, ***Jacob Teeter***, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; M. Sarker,* University of Nebraska - Lincoln*; C. Tao, J. Huang,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; W. Lu, J. Bernholc,* North Carolina State University*; A. Sinitskii,* University of Nebraska - Lincoln*; A. Li,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

The archetypical chevron-shape graphene nanoribbon (GNR) broke new ground in the on-surface synthesis of carbon-based nanomaterials with its development in 2010 by Cai *et al*[1]. Subsequent innovation predicated on this discovery introduced a wide variety of GNRs with differing shapes, edge types, heteroatomic substitutions, topological phases, and more. One drawback to studying GNRs arising from surface-assisted synthesis is the intrinsic electronic hybridization between the GNR and the surface upon which it was grown. This convolutes electronic characterization such as scanning tunneling spectroscopy (STS), but can be mitigated somewhat through tip-based manipulation of the GNRs onto an insulating layer on the surface, or by introducing a powder of solution-synthesized GNRs to a semiconducting substrate. Only recently has a method been developed - utilizing rutile TiO_2(011), rationally designed fluorinated precursors, and a

surface-assisted cyclodehydrofluorination reaction - to achieve bottom-up-synthesized atomically precise GNRs on such a surface[2].

In this work, we have developed more fluorinated precursors to expand the set of atomically precise GNRs grown on semiconducting surfaces and studied their assembly on Au(111) using scanning tunneling microscopy. In particular, we have produced and prototyped on Au(111) a fluorinated chevron precursor intended to yield chevron-type GNRs on TiO_2(011). With all other factors equivalent, the adsorption of the precursor is heavily dependent on the temperature of the surface of the Au(111) crystal on which it is deposited. The lack of adsorption at room temperature is in sharp contrast with the non-fluorinated precursor, which can be deposited at room temperature and post-annealed to produce GNRs in good yield. We attribute this discrepancy to interactions between the internal F atoms and the Au(111) surface, which is supported by theoretical calculations.

This research was performed at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility.

1.Cai, J.; Ruffieux, P.; Jaafar, R.; Bieri, M.; Braun, T.; Blankenburg, S.; Muoth, M.; Seitsonen, A. P.; Saleh, M.; Feng, X.; Müllen, K.; Fasel, R., Atomically precise bottom-up fabrication of graphene nanoribbons. Nature 2010, 466.

2.Kolmer, M.; Steiner, A.-K.; Izydorczyk, I.; Ko, W.; Engelund, M.; Szymonski, M.; Li, A.-P.; Amsharov, K., Rational synthesis of atomically precise graphene nanoribbons directly on metal oxide surfaces. Science 2020, 369 (6503), 571-575

5:20pm **NS2+AS+EM-WeA-10 STM Study of Superconducting Film FeTe(1-x)Se(x) on Topological Insulator Bi_2Te_3, *Hoyeon Jeon**, W. Ko, M. Brahlek, R. G. Moore II, A. Li,* Oak Ridge National Laboratory, USA

Topological superconductors (TSCs) have attracted great attention because they can host Majorana fermions for quantum computation. Because natural TSCs are rarely found, alternative ways to make TSCs are badly needed. One of them is using proximity effect by combining two-dimensional Dirac surface states of topological insulator (TI) with s-wave superconductivity (SC) to generate localized topological Majorana zero modes in vortex cores. Here we report the epitaxial growth of SC films of FeTe(1-x)Se(x) on TI of Bi_2Te_3, their electronic structures and surface inhomogeneities of superconductivity using scanning tunneling microscope/spectroscopy (STM/STS). A variety of samples are examined with different thicknesses of superconducting layer and selenium concentrations. We expect our results to be relevant for searching for materials platforms to host topological superconductivity.

The research is supported by the U.S. Department of Energy (DOE), Office of Science, National Quantum Information Science Research Centers., the Quantum Science Center (QSC), a National Quantum Information Science Research Center of the U.S. Department of Energy (DOE).

5:40pm **NS2+AS+EM-WeA-11 Atomic-Scale Mapping of Thermoelectric Properties of Noble Transition Metal Dichalcogenides*, Saban Hus**, A. Li,* Oak Ridge National Laboratory*; L. Liu, Y. Chen,* Purdue University

Monolayer noble transition metal dichalcogenides with hexagonal lattice structure are predicted to be high performance thermoelectric materials at room temperature [1]. Their pentagonal counterparts promise even better performance due to the in-plane anisotropy of the lattice [2]. However, like many other features of 2D materials, their thermoelectric properties can significantly be altered by the heterogeneities in the atomically thin layers [3]. Using a scanning tunneling microscope (STM), we investigate the thermoelectric properties of both pentagonal and hexagonal noble transition metal dichalcogenide monolayers in atomic resolution. We observe that atomic-scale defects and variations in 2D layer-substrate interface create a rich thermoelectric landscape invisible to mesoscopic scale measurements. Precise control and utilization of these heterogeneities can lead to next-generation thermoelectric devices and materials for energy applications.

[1] B. Marfoua and J. Hong, ACS Appl. Mater. Interfaces 11, 38819 (2019)

[2] D. Qin, et al., Sci. Reports. 8, 2764 (2018).

[3] S.M. Hus, A-P. Li, Progress in Surface Science 92, 176 (2017)

* This work was supported by Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

Quantum Information Science Focus Topic
Room 302 - Session QS+EM+MN+NS-WeA

Systems and Devices for Quantum Information

Moderators: Megan Ivory, Sandia National Laboratories, **Dave Pappas**, Rigetti Computing

2:20pm **QS+EM+MN+NS-WeA-1 Photonics-Integrated Microfabricated Surface Traps for Trapped Ion Applications*, Megan Ivory**, W. Setzer, N. Karl, J. Schultz, J. Kwon, M. Revelle, R. Kay, M. Gehl, H. McGuinness,* Sandia National Laboratories **INVITED**

Some of the more advanced quantum systems for applications spanning clocks, sensors, and computers are based on the control and manipulation of atoms.While these atomic systems have led to promising results in laboratory systems, the transition of these devices from the laboratory to the field remains a challenge.Recently, advances in compact vacuum technology, microfabricated surface traps, and integrated photonics are paving the way toward deployable solutions.Here, I discuss ongoing efforts at Sandia National Laboratories to leverage microfabricated surface traps for low size, weight, and power (SWaP) deployable trapped-ion systems, and the unique systematics presented by these integration efforts.In particular, I present initial demonstrations of trapped ions utilizing multilayered waveguides for UV and visible/IR light and single photon avalanche detectors integrated with microfabricated surface traps.I also present characterization of heating rates and frequency shifts in these integrated devices, and an outlook for further reducing SWaP via compact vacuum systems.

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3:00pm **QS+EM+MN+NS-WeA-3 Toward Heterogeneous Quantum Networks: Interfacing Trapped Ion, Superconducting, and Integrated Photonic Qubits*, Kathy-Anne Soderberg**, A. Paul,* Air Force Research Laboratory*; N. Barton, A. Brownell,* Murray Associates*; D. Campbell,* Air Force Research Laboratory*; C. Craft,* Technergetics*; M. Fanto, D. Hucul,* Air Force Research Laboratory*; A. Klug,* Griffiss Institute*; M. LaHaye,* Air Force Research Laboratory*; M. Macalik,* Booz Allen Hamilton*; K. Scalzi,* Technergetics*; J. Schneeloch,* Air Force Research Laboratory*; M. Senatore,* Griffiss Institute*; E. Sheridan,* National Academies of Sciences, Engineering, and Medicine*; D. Sica,* Griffiss Institute*; A. Smith, Z. Smith, C. Tison,* Air Force Research Laboratory*; C. Woodford,* Griffiss Institute **INVITED**

Effective and efficient ways to connect disparate qubit technologies is an outstanding challenge in quantum information science. However, the ability to interface different qubit modalities will have far-reaching implications for quantum computing and quantum networking. Here we present plans and progress toward interfacing trapped ion, superconducting, and integrated photonic qubits for the purpose of entanglement distribution in a quantum network. We will also discuss how this work connects to the AFRL distributed quantum networking testbed.

Approved for Public Release [Case number AFRL-2022-1621] Distribution Unlimited

4:20pm **QS+EM+MN+NS-WeA-7 Superconductor/Semiconductor Heterostructures for Quantum Computing Applications*, Chris Palmstrøm**,* University of California, Santa Barbara **INVITED**

Superconductor/semiconductor heterostructures have potential for quantum computing applications. Coupling superconductivity to near surface quantum wells (QW) and nanowires of high spin-orbit semiconductors have allowed the observation of zero bias peaks, which can be a signature of, but not proof of, Majorana Zero Modes, a key ingredient for topological computing. These results of induced superconductivity pave the way for lithographically defined complex superconductor/semiconductor nanostructured networks necessary for quantum computation.

Our efforts have focused on developing high mobility of near surface quantum wells of the high spin-orbit semiconductors InAs, InSb and $InAs_ySb_{1-y}$. Rather than relying on post growth lithography and top down

etching to form semiconductor nanostructures, we have investigated the development of shadow superconductor growth on atomic hydrogen cleaned MOVPE-grown vapor-liquid-solid InSb nanostructures and in-vacuum chemical and molecular beam epitaxy selective area grown InAs nanostructures. We have identified Sn as an alternative for Al for use as superconductor contacts to InSb vapor-liquid-solid nanowires, demonstrating a hard superconducting gap, with superconductivity persisting in magnetic field up to 4 Tesla. Further, a small island of Sn-InSb exhibits the two-electron charging effect, a clear indication of a supercurrent.

In more conventional superconductor qubits, a dramatic size reduction of the superconducting transmon devices is predicted by the development of merged element transmon devices based on superconductor/semiconductor/superconductor heterostructures. These superconductor/semiconductor/superconductor heterostructures also allow for selective control of conductance modes in planar lateral multi-terminal Josephson Junctions

In this presentation, progress in developing superconductor/semiconductor heterostructures for quantum computing applications will be presented. This will include progress in in-situ patterning and selective area growth, multi-terminal Josephson Junctions and the recent progress towards developing a Si fin based merged element transmon – the FinMET.

5:00pm **QS+EM+MN+NS-WeA-9 High Throughput Measurements of III-V Semiconductor Materials Stack of 2DEG-Based Tunable Couplers*, Nicholas Materise,*** Colorado School of Mines*; J. Pitten,* University of Colorado at Boulder*; W. Strictland,* New York University*; A. McFadden,* National Institute for Science and Technology (NIST)*; J. Shabani,* New York University*; E. Kapit,* Colorado School of Mines*; C. McRae,* University of Colorado at Boulder

Recent success in integrating cryogenic semiconductor classical systems with superconducting quantum systems promises to reduce the room temperature classical signal processing bottleneck. Incorporating semiconductor quantum devices with superconducting ones as tunable couplers and hybrid quantum systems requires quantitative estimates of the loss introduced by those devices. We report loss measurements of the III-V semiconductor stack used in 2DEG-based gatemon qubits and couplers using a superconducting microwave cavity. Extending the high throughput, low-cost substrate measurement method to thin films grown by molecular beam epitaxy, we can investigate surface roughness losses, bulk losses, and interface losses in a single microwave package. As with our previous measurements of substrates, we perform comparison studies with CPW resonators to validate our approach.

5:20pm **QS+EM+MN+NS-WeA-10 Strong Coupling between a Superconducting Microwave Resonator and Low-Damping Magnons Using Vanadium Tetracyanoethylene Thin Films*, Q. Xu, H. Cheung,*** Cornell University*; D. Cormode, H. Yusuf,* The Ohio State University*; Y. Shi,* University of Iowa*; M. Chilcote,* Cornell University*; M. Flatté,* University of Iowa*; E. Johnston-Halperin,* The Ohio State University*; **G. D. Fuchs**,* Cornell University **INVITED**

Hybrid quantum systems – in which excitations with distinct origin are hybridized through a resonant interaction – are attractive for quantum technologies because they enable tunability and the ability to combine desirable properties of each excitation. Here we study the hybrid excitation of a superconducting microwave resonator mode and a ferromagnetic resonance mode of vanadium tetracyanoethylene ($V[TCNE]_x$) thin films. Our work addresses a key challenge for hybrid superconducting resonator-magnon devices: the integration of a low damping thin-film material with microfabricated superconducting circuits. $V[TCNE]_x$ is a molecular-based ferrimagnet with exceptionally low magnetic damping – as low as 5×10^{-5} at room temperature. The ability to grow thin films of this material at low temperature via chemical vapor deposition and pattern it via lift-off processing enables the fabrication of integrated quantum magnon devices using this material. We couple a $V[TCNE]_x$ magnon mode to the mode of a thin-film Nb lumped-element LC resonator and demonstrate strong coupling, characterized by cooperativities in above 10^2. Characterization of this hybrid resonator-magnon system in both the frequency domain and the time domain reveals hybridization between resonator photons and magnons. This work demonstrates a pathway for scalable and integrated quantum magnonic technologies.

6:00pm **QS+EM+MN+NS-WeA-12 Role of Point Defect Disorder on the Extraordinary Magnetotransport Properties of Epitaxial Cd_3As_2*, Jocienne Nelson,*** *A. Rice, C. Brooks, I. Leahy, G. Teeter, M. van Schilfgaarde, S. Lany, B. Fluegel, M. Lee, K. Alberi,* NREL

Three-dimensional topological semimetals host extremely large electron mobilities and magnetoresistances making them promising for a wide range of applications including in optoelectronic devices, renewable energy, and quantum information. However, the extent to which disorder influences the properties of topological semimetals remains an open question and is relevant to both the understanding of topological states and the use of topological materials in practical applications. As a particular example, epilayers of the prototypical Dirac semimetal Cd3As2 exhibit high electron mobilities despite a having very high dislocation densities.[1,2]

Native point defects are inevitable in crystalline materials and introduce long and short-range disorder potentials that will impact carrier transport behavior. To understand their role in topological semimetals, we use molecular beam epitaxy to achieve unmatched and systematic control of point defect concentrations in Cd_3As_2. By reducing the concentration of scattering point defects, we increased the mobility from 5000 to 18,000 cm2/Vs and the magnetoresistance from 200% to 1000%. We find good agreement with the guiding center diffusion model, which indicates point defects are essential to the large linear magnetoresistance in topological semimetals.[3] However, the degree of linear magnetoresistance, is found to correlate inversely with measures of disorder. Our results demonstrate the importance of engineering high quality material with dilute concentrations of point defects to optimize the magnetoresistance properties in topological semimetals.[4]

[1] A.D. Rice, K. Park, E.T. Hughes, K. Mukherjee and K. Alberi, *Phys. Rev. Mater.*, **3**, 121201(R) (2019)

[1] M. Goyal, S. Salmani-Rezaie, T.N. Pardue, B. Guo, D.A. Kealhofer and S. Stemmer, *APL Mater.*, **8**, 051106 (2020)

[1] I.A. Leahy, Y.-P. Lin, P.E. Siegfried, A.C. Treglia, J.C.W. Song, R.M. Nandkishore and M. Lee*, PNAS*, **115**, 10570 (2018)

[1] J. N. Nelson, A. D. Rice, C. Brooks, I. A. Leahy, G. Teeter, M. Van Schilfgaarde, S. Lany, B. Fluegel, M. Lee, K. Alberi *arXiv:2206.10023* (2022).

2D Materials Technical Group
Room 303 - Session 2D+AS+NS+SS-ThM

2D Materials: Scanning Probe Microscopy and Spectroscopy

Moderators: Matthias Batzill, University of South Florida, **Yi-Ting Hsu**, University of Notre Dame

8:00am **2D+AS+NS+SS-ThM-1 Atomically Precise Graphene Nanoribbons for Quantum Electronics**, ***An-Ping Li,*** Oak Ridge National Laboratory **INVITED**

An-Ping Li, Chuanxu Ma, Marek Kolmer, Wonhee Ko, Kunlun Hong, Peter Bonnesen, Alex Puretzky, Jingsong Huang, Liangbo Liang, Bobby Sumpter

Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

Graphene nanoribbons (GNRs) possess high mobility and current-carrying capability, sizeable bandgap, long mean free path, localized spin and topological edges states [1]. These properties make them attractive candidates for quantum electronic applications. Atomically precise GNRs can be synthesized bottom-up using controlled on-surface chemical reactions from rationally designed molecular precursors [2]. The on-surface reactions of molecular precursors performed under ultra-high vacuum conditions can further be combined with scanning tunneling microscopy (STM) for in situ characterization of atomic, electronic, and magnetic properties. In this talk, I will discuss our recent progress in realizing novel quantum states in GNR heterostructures at atomic precision. First, a bottom-up approach is developed to couple graphene nanodot (GND) covalently at the edges of GNR to create quantum-well-like states for well-defined narrow-band light emission [3], which highlights a route to programmable and deterministic creation of quantum light emitters. Second, atomically precise GNRs are obtained by the on-surface synthesis approach on a model metal oxide, showing entangled magnetic states decoupled from the substrate [4]. These works illustrate that by using bottom-up synthesis—complemented by advanced microscopy and spectroscopy, as well as theory/simulation to enable atomistic level control—a rational approach to graphitic quantum electronic materials can be established with atomic precise.

The research was conducted at the Center for Nanophase Materials Sciences (CNMS), a US Department of Energy User Facility. The electronic characterization was funded by ONR grants N00014-20-1-2302 and N00014-16-1-3153.

[1] H. Wang et al., Graphene nanoribbons for quantum electronics, *Nat. Rev. Phys.* 3, 791 (2021). https://doi.org/10.1038/s42254-021-00370-x

[2] C. Ma et al., On-surface cyclodehydrogenation Reaction Pathway Determined by Selective Molecular Deuterations, Chemical Science 12, 15637 (2021). https://doi.org/10.1039/D1SC04908A

[3]C. Ma et al., Engineering Edge States of Graphene Nanoribbons for Narrow-Band Photoluminescence, *ACS Nano* 14, 5090 (2020). https://doi.org/10.1021/acsnano.0c01737

[4] M. Kolmer et al., Rational synthesis of atomically precise graphene nanoribbons directly on metal oxide surfaces, *Science* 369, 571 (2021). https://www.science.org/doi/10.1126/science.abb8880

8:40am **2D+AS+NS+SS-ThM-3 Band Gaps of Single-Layer Transition-Metal-Dichalcogenides Determined by Scanning Tunneling Spectroscopy**, ***Randall Feenstra,*** *G. Frazier, J. Lou,* Carnegie Mellon University*; Y. Pan, S. Foelsch,* Paul Drude Institute, Germany*; Y. Lin, B. Jariwala, K. Zhang, J. Robinson,* Penn State University

Using scanning tunneling spectroscopy at a temperature of 5 K, the electronic states of single-layer MoS_2 and WSe_2, grown on epitaxial graphene, have been investigated. Data is acquired utilizing a high-dynamic-range method in which the sample-tip separation is varied as a function of the sample-tip voltage (separation is decreased linearly as the magnitude of the voltage is reduced). Resulting spectra, when normalized to constant sample-tip separation, display conductance values that range over 5 – 6 orders of magnitude above the noise level [1]. The resulting edges of the conduction and valence bands, as well as onsets of higher/lower lying bands, are clearly defined. A theory for fitting the spectra is developed in which the varying wave-vector of the electronic states is explicitly included, yielding significant improvement in the quality of the fits compared to prior work [2]. Band onset energies can be determined with an accuracy of ~20 meV [1]. However, certain features in the data remain poorly explained by the model, in particular, an apparent broadening or smearing of the band edges which is 5x larger than that given by any instrumental effect (kT broadening together with modulation voltage of the measurement). Tentatively, this additional broadening is attributed to tip-induced band bending. Results of fitting which includes this effect will be described.

[1] R. M. Feenstra, G. R. Frazier, Yi Pan, St. Fölsch, Y.-C. Lin, B. Jariwala, K. Zhang, and J. A. Robinson, J. Vac. Sci. Technol. A **39**, 011001 (2021).P. Mårtensson and R. M. Feenstra, Phys. Rev. B **39**, 7744 (1989).

[2] H. M. Hill, A. F. Rigosi, K. T. Rim, G. W. Flynn, and T. F. Heinz, Nano Lett. **16**, 4831 (2016).

9:00am **2D+AS+NS+SS-ThM-4 Open-Source Controller for Scanning Probe Microscopy Applications**, *M. Kangül, N. Asmari Saadabad, M. Penedo,* ***Georg Fantner,*** École Polytechnique Fédéral de Lausanne, Switzerland

Transferring the outcomes of academic research into patented industrial products converts the conceptual proof into accessible and sustainable technology. However, it is not always beneficial for researchers; as scientific studies often push the limits of instruments, requiring custom functionalities. In order to resolve these needs, several options are available, among which, hacking off-the-shelf products or rebuilding a simple copy of the existing technology are the most common ones. Either of these solutions slows down the research in a multidisciplinary field like Scanning Probing Microscopy (SPM). To not be limited by the disadvantages of the aforementioned solutions, we have developed an open-source SPM controller as a technology that eases innovation in not only our research but also in the whole SPM community.

In this regard, we have chosen a modular design strategy. A commercial FPGA (NI-7856R) with embedded real-time controller code sits at the core of the controller hardware. An FPGA adapter board for the flexibility of choosing different FPGAs, interconnect boards to perform digitally controlled (SPI) analog signal conditioning, such as filters and gain-offset stages, and a microscope adapter board to easily customize the input/output terminals of the controller for various SPM instruments are the other components of the modular hardware design. To run the controller, a custom software suite was developed in the graphical programming language LabVIEW (National Instruments). Similar to hardware, the software is also implemented in a highly modular fashion. The functions have been formulated into separate modules with minimum cross-dependency to reduce the complexity of coding for new developers.

The interest of our scientific and industrial collaborators in adapting and using our SPM controller in their instruments has motivated us to put an extra effort into building supporting documentation and creating an open-source platform. For the hardware, the documentation comprises design files, manufacturing guides, and assembly notes. For the software, documentation explaining the functionality of the real-time controller is provided, while the user interface side of the software is documented with user guides.

Here we report an open-source modular SPM controller provided with detailed documentation on both hardware and software levels. Modularity and documentation make it an easy-to-adapt instrument for various SPM applications. This platform has already been successfully adapted to control different SPMs such as contact mode AFM, AM-AFM, high-speed off-resonance tapping mode AFM, scanning ion conductance microscope, correlative AFM/SEM, and STM.

9:20am **2D+AS+NS+SS-ThM-5 Activation of Resistive Switching in TaOx on the Nanoscale**, ***Olha Popova,*** ORNL

In present work we have shown two an alternative pathways to induce resistive switching of prototypical TaOx –(1) via direct biasing with a nanoscale AFM probe in oxygen free environment and (2) via He-ion patterning. Both approaches were carried out with fine control over the net amount of dissipated energy during activation. With direct AFM probe activation in oxygen free environment, we were able to switch conducting properties of the material in poorly controlled conditions. This is a similar pathway to electroforming, albeit combined with microscopy, which revealed directly the changes induced in the film during field-induced insulator-metal transition. Filamentary regions down to 20 nm in dimension could be routinely achieved by reducing the peak current during the activation cycle. Nevertheless, the process remains extremely stochastic. In contrast, by use of He ion irradiation pristine insulating state can be easily converted to conducting and resistively switching state without any breakdown, but the transition itself is a smooth function of

ion-irradiation dose. These findings revealed numerous intermediate states of TaOx can be created by controlled ion-irradiation. Remarkably, this effect is directly compatible with device architectures, potentially allowing for a high-degree of on-demand tunning of neuromorphic circuitry and materials. By combining AFM and SEM-CL we were able to determine dependence of the ion dose/materials damage correlated with the chemical, structural and compositional tunability of thin TaOx films which offers significant opportunities to neuromorphic nanoelectronic materials in comparison with more mature technologies based on traditional bulk electronic materials.

9:40am **2D+AS+NS+SS-ThM-6 Probing Sub-Nanoscale Photophysical and Photochemical Processes via Localized Surface Plasmons: Vibrational Nano-Spectroscopy**, ***Sayantan Mahapatra***, *N. Jiang,* University of Illinois - Chicago

Conventional spectroscopic techniques are limited by the optical diffraction limit to about half wavelength and therefore offer about 200 nm x 200 nm microscopic zone for working in the visible light range. Tip-enhanced Raman spectroscopy (TERS) emerges as an advanced analytical technique, where the plasmonically active probe is not only used to detect the tunneling current but also to interrogate the local chemical environment of the surface adsorbed molecules with angstrom scale precision. In this work, we report a topological and chemical analysis of two regioisomers (positional isomers), trans- and cis-tetrakispentafluorophenylporphodilactone (trans- and cis-H_2F_{20}TPPDL) by scanning tunneling microscopy (STM), ultrahigh vacuum (UHV) TERS on Ag(100) with the spatial resolution down to 8 Å, which has a wide range of applications in various field of surface science & nanotechnology such as regioselective catalysis reaction, chemical reactions, molecular electronics, etc. We have shown that it is possible to distinguish these two structurally very similar forms with high accuracy & precision. The two-component molecular junction has been identified using high resolution two-dimensional (2D) Raman mapping. Furthermore, the nanoscale molecule-substrate interactions have been addressed at the single-molecule level by employing different single-crystals i.e., Ag(100), Cu(100), and Au(100). Strong surface interactions at Cu(100) surface converted the flexible porphodilactone structure inverted, which was further verified by STM. In another case, the chemical transformation of adsorbed ferrocene dicarboxylic acid molecule was also analyzed via TERS on Cu(100) due to significantly strong interaction. Apart from the Raman signal enhancement, the highly energetic localized surface plasmons generated at the tip apex were utilized for site-selective C—Si bond activation inside a single 5,10,15,20-(tetra-trimethylsilylethynyl)porphyrin molecule. The nano-confined plasmonic field dissociated only one chemical bond, in presence of multiple chemically equivalent bonds inside the single molecule. To this end, multiple sites were also activated one by one and different types of products were visualized which could prove extremely useful in plasmon-induced site-selective heterogeneous catalysis application.

11:00am **2D+AS+NS+SS-ThM-10 Visualize Emergent Electron Orders in Two-Dimensional Quantum Materials**, ***Xiaomeng Liu***, Princeton University **INVITED**

Recent developments have enabled scientists to isolate various 2D materials and assemble them into van der Waals heterostructures with elaborate stacking and alignments. These van der Waals materials, constructed layer-by-layer, host numerous novel quantum phases. However, most studies so far are done by electrical transport measurements, lacking spatial and energy resolution. Scanning tunneling microscopes (STM) can provide unique insights to these emergent quantum phases by visualizing the electron wave function in real space. Using our recent study of the graphene quantum Hall system as an example, I will demonstrate using STM techniques to identify broken symmetries, visualize electron wavefunctions, and imaging quasiparticles.

11:40am **2D+AS+NS+SS-ThM-12 Reconstruct the Intrinsic Force Landscape of Interfacial Interaction with Excitation-Enhanced Force Spectroscopy**, ***Alan Liu***, *T. Sulchek,* Georgia Institute of Technology

The advancement of sensitive force transducers has enabled scientists to measure the subtle forces of interactions between molecules and interfaces at nanometer scales. Force spectroscopy techniques, such as dynamic force spectroscopy (DFS), extract a single representative force from each measurement, and require thousands of measurements with model assumptions to extract useful physical parameters of the interaction. This process is not only time consuming, but also the preciseness of the results relies largely on model assumptions, which make the results highly variable and dependent on experimental conditions. Furthermore, because DFS models presume the interaction to be a reversible reaction under certain energy/force landscape, parameters extracted by DFS method can only represent the rough shape of interaction landscape but not able to probe the detail landscape of underlying intrinsic interactions. Using our recently developed force spectroscopy framework[1], we can obtain the definitive intrinsic force landscape using a high sampling rate (above 1 MHz) atomic force microscopy (AFM) measurement. While most studies deemed the "snap" of AFM force measurement as an instantaneous action, we successfully sampled the fluctuation and real-time movement of the AFM probe at snap under a high sampling rate. At the snap location of each AFM force-distance measurement, transition points can be identified that define the bound state (or probe-in-contact state) and unbound state (or free oscillation state). Sampling at these transition points are key to probe the normally inaccessible portion of force landscape where the intrinsic force landscape has higher force gradient than the stiffness of the force probe. Next, we demonstrated how to modulate the snap locations of the force-distance curves by tuning the bandwidth of the excitation applied to the AFM probe. Lastly, we integrated the definitive forces sampled at various locations to reconstruct the intrinsic force landscape of the interaction without any model assumption or curve fitting process.

[1] Alan Y. Liu and Todd A. Sulchek, Reconstructing the Intrinsic Potential Energy Landscape of Interfacial Interactions with Thermally Modulated Force Spectroscopy, Phys. Rev. Res. 3, (2021).

12:00pm **2D+AS+NS+SS-ThM-13 AVS Graduate Research Awardee Talk: True Atomic-Resolution Imaging under Ambient Conditions via Conductive Atomic Force Microscopy**, ***Saima Sumaiya***[1], *M. Baykara,* University of California, Merced

Atomic-scale characteristics of surfaces dictate not only the governing principles of numerous scientific phenomena ranging from catalysis to friction, but also the design and performance of billions of state-of-the art nanoscale devices ubiquitous in modern life. Despite such an enormous significance, our ability to visualize surfaces on the atomic scale is severely limited by the strict conditions under which the related methods are operated. In particular, the two prominent methods utilized to achieve atomic-resolution imaging – scanning tunneling microscopy (STM) and noncontact atomic force microscopy (NC-AFM) – are typically performed under ultrahigh vacuum (UHV) and often at low temperatures. Perhaps more importantly, results obtained under such well-controlled, clean environments bear little relevance for the great majority of processes and applications that often occur under ambient conditions. Therefore, a method which is able to reliably and robustly image surfaces with atomic-level spatial resolution under ambient conditions can be regarded as a "holy grail" of surface science. Here, we first show that the method of conductive atomic force microscopy (C-AFM) can be utilized to achieve true atomic-resolution imaging under ambient conditions by imaging single atomic vacancies on molybdenum disulfide (MoS_2), without any control over the operational environment or elaborate sample preparation. With our method, we are also able to image several other types of defects on MoS_2, demonstrating that C-AFM can be utilized to investigate surface defects in a reliable, straightforward fashion under ambient conditions, in contrast to the often extensive operational requirements of STM and NC-AFM. We further employ the method of C-AFM to record atomic-resolution images on different classes of materials such as gold (metal), WSe_2 (semiconductor), $PtSe_2$ (semimetal), and α-Mo_2C (metallic transition metal carbide), proving its versatility in terms of the material classes it can be applied to. Our approach overcomes many of the classical limitations associated with STM and NC-AFM, and the findings herald the emergence of C-AFM as a powerful tool for atomic-resolution imaging under ambient conditions.

[1] **AVS Graduate Research Awardee**

Quantum Information Science Focus Topic
Room 302 - Session QS+AP+EM+MN+NS+SS-ThM

Systems and Devices for Quantum Computing

Moderators: Vivekananda Adiga, IBM, T.J. Watson Research Center, **Kathy-Anne Soderberg**, Air Force Research Laboratory

8:00am **QS+AP+EM+MN+NS+SS-ThM-1 Effects of Environmental Radioactivity on Superconducting Qubits**, *L. Cardani,* ***Ambra Mariani,*** Istituto Nazionale di Fisica Nucleare, Italy **INVITED**

Environmental radioactivity was recently discovered as a potential limit for superconducting quantum bits.

We review recent works proving that ionizing radiation lowers the coherence of singe qubits and induces correlated errors in qubits arrays. We also present preliminary studies showing that operating qubits in a low-radioactivity environment improves their performance. These results fuelled the interest of several European and US groups in further investigating and mitigating radioactivity for next-generation quantum processors.

Using radioactivity measurements and simulations, we estimated the separate contribution of “far” radioactive sources (cosmic rays and laboratory radioactivity) and close materials contamination (chip holder, magnetic shield, …) on a typical chip, focussing on a qubit prototype developed within the SQMS center. We present such contributions and discuss the possibility of mitigating them in "standard" qubit laboratories or, eventually, in deep underground facilities.

8:40am **QS+AP+EM+MN+NS+SS-ThM-3 Dynamics of a Dispersively Coupled Transmon in the Presence of Noise from the Control Line**, ***Antti Vaaranta,*** Bluefors Oy, Finland*; M. Cattaneo,* University of Helsinki, Italy*; R. Lake,* Bluefors Oy

In this talk we present theoretical results from a complete description of transmon qubit dynamics in the presence of noise introduced by an impedance-matched resistor (50 Ohm) that is embedded in the qubit control line, acting as a noise source [1]. We derive a model to calculate the qubit decoherence rate due to the noise emanating from this noise source [2]. The resistor is treated, using the Caldeira-Leggett model, as an infinite collection of harmonic LC-oscillators making it a bosonic bath [3]. To obtain the qubit time evolution affected by this remote bath, we start with the microscopic derivation of the Lindblad master equation using the dispersive Jaynes-Cummings Hamiltonian with added inductive coupling to the bath. To solve the resulting master equation, we transform it into a block diagonal form by exploiting its underlying symmetries following Ref. 4. The block diagonalization method reveals that the long time decoherence rate is given by the slowest decaying eigenmode of the Liouvillian superoperator. Moreover, when the readout resonator is in the equilibrium thermal state, the rate of exponential decoherence of the qubit is almost exactly exponential for all times with the predicted rate given by the slowest decaying eigenmode. We also study how the decoherence rate depends on the temperature of the noise source and explore the strong and weak dispersive coupling regimes. The model captures the often used dispersive strong limit approximation of the qubit decoherence rate being linearly proportional to the number of thermal photons in the readout resonator. However, in the dispersive weak limit we predict remarkably better decoherence rates. The model parameters are completely determined by the values of the circuit components, allowing for the exact study of the dynamics on the level of each individual circuit element.

[1] S. Simbierowicz et al., Rev. Sci. Instrum. 92, 034708 (2021).

[2] A. Vaaranta, Study of environmental effects on a dispersive transmon qubit, MSc thesis, Univ. of Helsinki, (2022).

[3] M. Cattaneo and G. Paraoanu, Adv. Quantum Technol. 2100054 (2021).

[4] M. Cattaneo et al., Phys. Rev. A 101, 042108 (2020).

9:00am **QS+AP+EM+MN+NS+SS-ThM-4 Accurate Microwave Characterization for Superconducting Quantum Technology**, ***Slawomir Simbierowicz,*** Bluefors Oy, Finland

Recent breakthroughs in quantum technology have highlighted a need for methods for accurate characterization of cryogenic microwave devices at millikelvin temperatures. In this two-part talk, I will highlight recent progress on microwave measurements at the quantum device reference plane including: (1) system noise characterization of amplifier chains, and (2) calibrated S-parameters of qubit drive line components.In the first part, I will discuss an impedance-matched variable temperature noise source which can be installed in a coaxial line of a cryostat. Using the method of hot/cold source with many input noise temperature points, the system noise temperatures of qubit readout amplifier cascades can be determined. I present measurement results in terms of added noise in Kelvins or photons from a four-wave (4WM) mixing traveling wave parametric amplifier (TWPA) [1], a Josephson parametric amplifier [2], 3WM TWPA, and high electron mobility transistor amplifiers [1].In the second part of the talk, I will present measurements of the 1-port S-parameters of qubit drive line components using a data-based short-open-load calibration at a temperature of 30 mK [3]. The measurement enables us to model systematic errors in qubit state preparation due to non-idealities in qubit control lines such as impedance mismatch. We model the results using a master equation simulation of all XY gates performed on a single qubit. Our work directly addresses the gap between electrical engineering parameters of individual measurement components and performance of the quantum device itself.

REFERENCES

[1] Slawomir Simbierowicz, Visa Vesterinen, Joshua Milem, Aleksi Lintunen, Mika Oksanen, Leif Roschier, Leif Grönberg, Juha Hassel, David Gunnarsson, and Russell E. Lake, "Characterizing cryogenic amplifiers with a matched temperature-variable noise source", Rev. Sci. Instr. **92**, 034708 (2021)

[2] Mustafa Bal et al., “Overlap junctions for superconducting quantum electronics and amplifiers”, Appl. Phys. Lett. **118**, 112601 (2021)

[3] Slawomir Simbierowicz, Volodymyr Y. Monarkha, Suren Singh, Nizar Messaoudi, Philip Krantz, and Russell E. Lake, "Microwave calibration of qubit drive line components at millikelvin temperatures", Appl. Phys. Lett. **120**, 054004 (2022)

9:20am **QS+AP+EM+MN+NS+SS-ThM-5 Improving Qubit Performance Through Engineering of the Substrate-Josephson Junction Interface**, ***Cameron Kopas****, H. Cansizoglu, R. Cochrane, B. Ercan,* Rigetti Computing*; D. Goronzy, C. Torres-Castanedo,* Northwestern University*; J. Oh,* Ames Laboratory*; A. Murthy,* Fermi Lab*; E. Lachman,* Rigetti Computing*; A. Romanenko, A. Grassellino,* Fermi Lab*; M. Kramer, L. Zhou,* Ames Laboratory*; M. Bedzyk,* Northwestern University*; J. Mutus,* Rigetti Computing*; M. Hersam,* Northwestern University*; K. Yadavalli,* Rigetti Computing **INVITED**

The performance of a superconducting qubit is often limited by dissipation and two-level systems (TLS) losses. The dominant sources of these losses are believed to come from interfaces and surfaces, likely as a result of fabrication processes, materials, or atmospheric exposure. We show that certain chemical surface treatments can be used to modify the silicon surface before Josephson junction deposition, reducing the number of strongly-coupled TLS, and improving T1. While identifying specific microscopic sources for loss and TLS is still an open question, targeted characterization of test structures will show which physical changes correlate with performance improvements. We report chemical, structural, and low-temperature microwave characterization of superconducting qubits and films fabricated with different Si surface treatments.

11:00am **QS+AP+EM+MN+NS+SS-ThM-10 Design and Optimal Control of Superconducting Qubits to Achieve Quantum Speed Limits**, ***Meenakshi Singh,*** Colorado School of Mines, USA **INVITED**

Fast two-qubit entangling gates are essential for quantum computers with finite coherence times. The finite interaction strength between qubits introduces a theoretical speed limit on the speed of these two-qubit entangling gates. This speed limit has been analytically found only for a two-qubit system under the assumption of negligible single qubit gate times. Here, we demonstrate such a speed limit experimentally using optimal control on two superconducting transmon qubits with a fixed capacitive coupling and finite single qubit gate times. Furthermore, we investigate the effect of additional couplings on the speed limit, both through introduction of an ancillary qubit as well as through utilization of higher transmon energy states. Finally, we discuss the generalization to many qubit systems where properly leveraging all available couplings can provide dramatic speedups.

11:40am **QS+AP+EM+MN+NS+SS-ThM-12 Atomic Scale Processing for Quantum Computing**, ***Harm Knoops,*** Oxford Instruments Plasma Technology, Netherlands **INVITED**

With the increasing technological readiness of quantum technology (QT) the field has to start focussing on scalable fabrication methods for

quantum bits (qubits) and quantum circuits. This contribution will focus on the enabling role atomic scale processing (ASP) methods such as atomic layer deposition (ALD) and atomic layer etching could play in scaling of QT. The main focus will relate to superconducting qubits and processing of superconducting nanolayers.

Superconducting nanolayers (metals, metal-nitrides) are required for various roles in QT including use in resonators, single-photon detectors, and interconnects.[1] The electrical contacts needed to control the qubits will require non-planar connectivity using superconducting interconnects.[2]Adequate routes for fabrication of planar superconducting layers exist, but for 3D interconnects or through-silicon vias (TSVs), the excellent conformality of ALD nanolayers could be essential. Although for resonators conformality is not a challenge, ALD's thickness control and uniformity should allow high-quality resonators with low spread in properties. For these superconducting nanolayers, metal-nitride compounds have been identified as particularly promising since they exhibit limited surface oxidation (compared to pure metals such as Nb), combined with relatively high critical temperature (T_c) for superconductivity (e.g., as compared to Al). Despite the challenges that the synthesis of high-quality nitrides pose, plasma ALD has demonstrated the capability to deposit high-quality nitrides (e.g., low O content, high electrical conductivity).[3] Furthermore, substrate-biased plasma-ALD offers unique opportunities to obtain and tune high-quality nitrides.[4] For removal of surface oxides or smoothing of resonator surfaces and interfaces, approaches combining ALD and ALE could be of interest.[5] Both ALD and ALE are envisaged to be key tools to allow scaling of these devices and advance the QT field.

References

1. Giustino et al., *J. Phys. Mater.***3**, 042006 (2021)
2. Kjaergaard et al., *Annu. Rev. Condens. Matter Phys.***11**, 369 (2020)
3. Knoops et al., *J. Vac. Sci. Technol. A***37**, 030902 (2019)
4. Faraz et al., *ACS Appl. Mater. Interfaces***10**, 13158 (2018)
5. Chittock et al, *Appl. Phys. Lett.* **117**, 162107 (2020)

Applied Surface Science Division
Room 320 - Session AS+2D+EM+MS+NS+SS+TF-ThA

Probing Defects at Surfaces and Interfaces

Moderators: Michaeleen Pacholski, The Dow Chemical Company, **Zachary Robinson**, SUNY Brockport

2:20pm **AS+2D+EM+MS+NS+SS+TF-ThA-1 Controlling InP Quantum Dot Surface Defects Using ALD-inspired Surface Chemistry and Phosphorus Kα and Kβ X-ray Emission Spectroscopy***, **Nayon Park,*** University of Washington **INVITED**

Colloidal InP quantum dots are a leading heavy-metal-free semiconductor material for spectral downconversion in current generation display technologies and future generation energy efficient LEDs. Achieving the brightest and narrowest photoluminescence (PL) relies on the synthesis of structurally and electronically defect-free quantum dots. InP quantum dots' high propensity for oxidation and the inherent oxidative defects arising from commonly used synthesis methods therefore motivates a systematic approach to probe InP oxidation as a function of synthesis and surface treatments and correlation with the resultant optical properties. Phosphorus X-ray Emission Spectroscopy (XES) presents itself as an exceptional tool in this regard. In this talk, I will show recent results from computational modeling where we find that native InP surface oxides give rise to dark states near the band edge. Replacing the surface indium with zinc to form a monolayer ZnO shell results in the reduction of dark states. Using ALD-inspired successive ionic layer adsorption and reaction (SILAR), we developed the colloidal, layer-by-layer growth strategy of metal oxide shells (i.e. ZnO, CdO, GaO_x, AlO_x) on InP quantum dots at room temperature using common ALD precursors (*i.e.*, metal alkyls and water). Metal oxide-shelled InP QDs generally show enhanced PL and evidence of bulk and local structural perturbations arising from the metal oxide as determined by X-ray diffraction and X-ray absorption spectroscopy. Further, we explore the impact of these metal oxide interfaces on the PL QY and emission linewidth of InP/ZnSe core/shell QDs. Upon growing a thin ZnSe shell, we observe improved PL properties, which we hypothesize to be attributable to the inhibition of phosphorus migration to the shell due to the presence of the metal oxide interlayer, as supported by X-ray emission spectroscopy. Taken together, these results suggest a clear path forward in the control and design of complex QD interfaces with atomistic insight for optoelectronic technologies.

3:00pm **AS+2D+EM+MS+NS+SS+TF-ThA-3 Characterization of MAX Phases using a Combination of Micro-spot XPS, HAXPES and C60 Cluster Depth Profiling***, **Kateryna Artyushkova,*** Physical Electronics USA*; M. Anayee, Y. Gogotsi,* Drexel University

Two-dimensional (2D) transition metal carbides, carbonitrides, and nitrides (MXenes) have seen significant increases in the number of research areas and publications. MXenes have a unique combination of properties that have led to many applications.[1] MXenes are usually synthesized by etching "A" layers that interleave "MX" layers in the bulk MAX precursors. MAX are represented by Mn+1AXn, where M denotes early transition-metals (Ti, V, Cr, Mo, etc.), X is N or C, and A is an A-group element such as Al, Si and others. During synthesis, impurities and defects may be introduced, which significantly impact the properties of the resulting materials. It is therefore critical to detect and quantify these defects and impurities.

X-ray Photoelectron Spectroscopy (XPS) has the advantages of being easily quantifiable and providing chemical information such as surface termination and oxidation. However, there are many challenges in using XPS for analyzing MAX and Mxene. The first is a very small size of MAX, less than a few tens of microns. With the development of focused scanning micro-probe X-rays, these limitations can be overcome. The other challenge is the extreme surface sensitivity of XPS. It is challenging to separate surface adventitious carbon and oxygen from possible oxygen incorporation in the carbon site. Depth profiling using a monatomic Ar ion beam is not suitable as it can introduce damage to the structure of MAX.

In this work, we are presenting two approaches to address this challenge. The first involves the application of Hard X-ray Photoelectron Spectroscopy (HAXPES), in which a monochromated Cr X-ray source is used to probe ~3 times deeper than a soft Al X-ray. The second utilizes a cluster ion gun source, such as C60, for damage-free depth profiling through individual MAX particles using ~8µm X-ray spot for probing if oxygen is present in the MAX structure.

3:20pm **AS+2D+EM+MS+NS+SS+TF-ThA-4 Unusual Trend in Thermal Stability of Alanine Different Ni Surfaces***, J. Ontaneda,* Queen Mary University of London, UK*; R. Grau-Crespo,* University of Reading, UK*; **Georg Held,*** Diamond Light Source, UK

Chirally modified heterogeneous catalysts promise massive savings of cost and toxic waste in the production of enantiopure precursors for high-value chemicals such as pharmaceuticals, fertilizers, or fragrants [1]. A key aspect is the thermal stability of chiral modifiers, which generally are chiral organic molecules bound to a chemically active metal surface. The enantioselective hydrogenation of methylacteoacteate (MAA) is a topical reaction, which is catalysed by nickel modified with chiral carboxylic acids, such as alanine, tartaric acid, or aspartic acid [2]. The components of this catalytic system have been investigated using various surface sensitive techniques [3,4,5]. Here we present a study of the thermal stability of alanine on the three most common Ni surfaces, {111}, {100}, and {110}, using synchrotron-based temperature-programmed photoelectron spectroscopy and X-ray absorption spectroscopy. In contrast to common experience with smaller molecules, alanine is more stable on the more open {110} and {100} surfaces compared to {111}. Comparison with a detailed DFT study identifies structural and electronic effects that play a role in this unusual behaviour.

References:

[1] G. Held and M. J. Gladys, Topics in Catalysis 48 (2008) 128 – 136.
[2] Izumi, Y., Adv. Catal. 1983, 32, 215−271.
[3] Keane, M. A., Langmuir 1994, 10, 4560−4565.
[4] P. Tsaousis, et al., J. Phys. Chem. C 122 (11) (2018) 6186 – 6194.
[5] R. E. J. Nicklin, et al., J. Phys. Chem. C 122 (2018) 7720 – 7730.
[6] W. Quevedo, et al., Langmuir 36 (2020) 9399 – 9411.

3:40pm **AS+2D+EM+MS+NS+SS+TF-ThA-5 Correlative Theoretical and Experimental Study of the PC | X Interfacial Bond Formation (X = TiN, AlN, TiAlN) During DC Magnetron Sputtering***, **Lena Patterer,*** *P. Ondračka, D. Bogdanovski, S. Karimi Aghda, J. Schneider,* Materials Chemistry, RWTH Aachen University, Germany

Due to their outstanding oxidation and wear resistance, cubic (Ti,Al)N is widely used as protective coatings on forming and cutting tools. These characteristics make (Ti,Al)N also an attractive candidate for the protection of polymer components. The composition-induced changes in the interfacial bond formation of DC magnetron sputtered TiN, AlN, and $Ti_{0.25}Al_{0.25}N_{0.5}$ onto polycarbonate (PC) substrates are systematically investigated by correlating theory and experiment. In order to simulate the sputtering condition by *ab initio* molecular dynamics, a periodic structural model of bulk PC consisting of 394 atoms was bombarded by several Ti, Al, and N atoms with a kinetic energy of 1 eV. While both Ti and N atoms show high reactivity towards all functional groups of the polymer during the surface bombardment, Al atoms selectively react only with the carbonate group of PC or other reactive functional groups that have formed during previous bombardment events (e.g. C-N groups). At the PC | TiN and PC | TiAlN interfaces, Ti and N contribute equally to the interfacial bond formation, whereas the PC | AlN interface is defined mostly by C–N groups with Al-rich clusters forming on top of these groups. X–ray photoelectron spectroscopy data of the PC | X interfaces (X = TiN, AlN, TiAlN) show a very good agreement with the above-discussed predictions as the formation of C-N, C-(Ti,Al), and (C–O)–(Ti,Al) bonds is experimentally verified. This shows that the here employed computational strategy enables predictions of the interfacial bond formation between polycarbonate and metal nitrides, and it is reasonable to assume that the here proposed research strategy can be readily adapted to other polymer | inorganic material interfaces.

4:00pm **AS+2D+EM+MS+NS+SS+TF-ThA-6 Using Resonant Photoemission Spectroscopy to Probe the Electronic Structure of Complex Oxides with Elemental and Orbital Specificity***, **Jessica McChesney,*** *D. Fong, H. Hong,* Argonne National Laboratory, USA

Understanding the role of defects and interfaces is necessary in order to realize many of the promising novel properties of complex oxide heterostructure devices. To this aim, we employ resonant angle-resolved photoemission spectroscopy to probe the electronic structure with elemental and orbital specificity of complex oxide heterostructure $LaTiO_3/SrTiO_3$ (LTO/STO).Combining these spectroscopy measurements with in-situ growth characterization we are able to determine the minimum thickness required to achieve high quality heterostructures with abrupt interfaces and to correlate the formation with the 2DEG with the

interface termination LTO/STO vs STO/LTO.In addition, we explore the role of oxygen vacancies in formation of the 2DEG on the bare substrate and reveal that contrary to expectations, the 2DEG is Ti^{4+} in character while the oxygen defects are Ti^{3+} in character.

Electronic Materials and Photonics Division
Room 304 - Session EM+AS+EL+NS+SS-ThA

Interfaces and Defect Engineering in Electronic & Photonic Materials & Devices

Moderator: Erin Cleveland, U.S. Naval Research Laboratory

2:20pm **EM+AS+EL+NS+SS-ThA-1 Design and Control of Defect-Mediated Properties in Electronic Ceramics***, **Elizabeth Dickey**,* Carnegie Mellon University **INVITED**

Crystalline lattice defects, e.g. vacancies, interstitials or substitutional ions, play an important role in the conductivity and dielectric properties of electronic ceramics. The material "defect chemistry" can be tuned to optimize the electronic and ionic conductivities for particular applications via doping, oxygen-activity and temperature control during processing. Beyond controlling the majority defect (carrier) concentrations, it is also important to control the minority defect concentrations as these can be especially relevant to the time-dependent electrical behavior. For example, applied electric fields in device applications provide a strong driving force for the electromigration of charged lattice defects. Furthermore, external conditions such as humidity, which can lead to proton incorporation, can also strongly influence time-dependent material properties. This talk will review our current understanding and implications of point defect equilibria, partial equilibria and dynamics in several prototypical electronic ceramics. Recent efforts to effectively co-dope dielectric materials to improve simultaneously limit both the electronic and ionic conductivity will be discussed.

3:00pm **EM+AS+EL+NS+SS-ThA-3 In-Situ Investigation of the Interface Formation between Si-Terminated Diamond and a NbxOy Electron Acceptor Layer for Electronic Applications***, **Gabrielle Abad**, P. Hopkins, S. McDonnell,* University of Virginia

Ultra-wide band gap semiconductors present one avenue for the next generation of semiconductor devices. Diamond, specifically, has shown promise in high power, frequency, and temperature electronics; however, issues with impurity doping has limited the development of diamond-based devices. Instead, surface charge transfer doping (SCTD), which avoids introduction of foreign atoms into the diamond lattice, has been used for inducing a two-dimensional hole gas at the diamond surface thus increasing its conductivity. The established method to achieve SCTD is to hydrogen-terminate the diamond surface prior to the addition of an electron acceptor layer; however, the degree of SCTD induced by H-termination is largely dependent on atmospheric exposure. Alternatively, silicon-termination of the diamond surface has been shown to produce the ordered surface with the negative electron affinity necessary for the SCTD mechanism. In this work, we investigate the combination of Si-terminated diamond with a Nb_xO_y electron acceptor layer, wherein we focus on understanding interface formation and chemistries, as well as elucidating if the band alignment mechanism is responsible for SCTD for this material system. Ultra-high vacuum (UHV) electron beam (e-beam) deposition of Si onto diamond substrates was carried out, followed by UHV annealing to produce the Si-terminated (100) diamond surface. X-ray photoemission spectroscopy (XPS) of core-level and valence band spectra was used to analyze chemical composition. To form the electron acceptor layer, Nb films were e-beam deposited onto the Si-terminated diamond surface by depositing Nb under varying oxygen partial pressures. XPS was used to observe how interfacial chemistry, electronic structure, and band alignment evolve with different Nb_xO_y compositions. The air stability of the electron acceptor layers was also investigated after atmospheric exposure via XPS. Analysis of the valence band spectra shows that band alignment would not result in SCTD for the Nb_xO_y/Si/diamond material system.

3:20pm **EM+AS+EL+NS+SS-ThA-4 Effects of Atmospheric UV-O_3 Exposure of WSe_2 on the Properties of the HfO_2/WSe_2 Interface***, **Maria Gabriela Sales**,* University of Virginia*; A. Mazzoni,* University of Maryland College Park*; W. Sarney,* Army Research Laboratory*; J. Pearson,* University of Maryland College Park*; S. Najmaei,* Army Research Laboratory*; S. McDonnell,* University of Virginia

Transition metal dichalcogenides (TMDCs) are a class of two-dimensional (2D) layered materials, in which each layer is held in-plane by strong chemical bonds, but held in the out-of-plane direction by weak van der Waals forces. For integration in an electronic device, TMDCs are typically capped in the gate region with a high-quality dielectric layer, where ultrathin (sub-5 nm) dielectric thicknesses are desired in order to achieve sufficient gate to channel electrostatic coupling. The unreactive basal plane of TMDCs makes atomic layer deposition (ALD) of dielectric films directly on top of these 2D materials challenging. In this work, we investigate the effects of atmospheric ultraviolet-ozone (UV-O_3) exposures of WSe_2 and use the UV-O_3 functionalized WSe_2 surfaces as substrates for ALD of HfO_2. We report two UV-O_3 functionalization regimes observed on WSe_2: lower exposure times, which do not result in oxidation of the WSe_2 surface, and higher exposure times, which result in a tungsten oxyselenide top layer. The properties of this oxidized layer, such as its thickness, structure, air stability, and thermal stability, are also investigated. Additionally, we note that both functionalization regimes result in variably doped WSe_2. We report on the interface chemistry observed after subsequent ALD of HfO_2, as measured with X-ray photoelectron spectroscopy (XPS). We note that variable, depth-sensitive doping states are found in the WSe_2 functionalized with higher exposure times. We also study the resultant morphologies of our deposited HfO_2 films with atomic force microscopy (AFM), and we find that both of our UV-O_3 functionalization regimes result in uniform and smooth HfO_2 films directly deposited by ALD. With the different functionalization regimes (with different interface chemistries) all providing uniform dielectric film deposition, our atmospheric UV-O_3 exposure technique on WSe_2 presents unique tunability and flexibility in the design of interfaces in devices.

3:40pm **EM+AS+EL+NS+SS-ThA-5 Near Zero Field Magnetoresistance and Electrically Detected Magnetic Resonance Studies of Instabilities in Semiconductor/ Insulator Systems***, **Patrick Lenahan**,* Pennsylvania State University **INVITED**

We have utilized both electrically detected magnetic resonance(EDMR) and near zero field magnetoresistance (NZFMR) spectroscopy to investigate the physics involved in instabilities such as stress induced leakage currents and time dependent dielectric breakdown in Si/SiO_2 and SiC/ SiO_2 systems. Both techniques are extremely sensitive and extend the sensitivity of conventional electron spin based techniques down to near nanoscale device structures. We find that the very simple spin-based NZFMR technique has significant analytical power in these investigations. The NZFMR studies can complement the more established EDMR measurements with simple and relatively inexpensive apparatus.

Fundamental Discoveries in Heterogeneous Catalysis Focus Topic
Room 321 - Session HC+AS+NS+SS-ThA

Special Session and Reception for the HC Community and to Celebrate Robert Madix

Moderators: Liney Arnadottir, Oregon State University, **Dan Killelea**, Loyola University Chicago, **Jason Weaver**, University of Florida

2:20pm **HC+AS+NS+SS-ThA-1 Gaede-Langmuir Award Talk: Not a Divide - A Continuum: Surface Science to Heterogeneous Catalysis***, **Robert J. Madix**[1],* Harvard University **INVITED**

The science of surface reactivity demands control of surface structure and surface composition. Surface science methods thus enable the investigation of reactions, including oxidations, hydrogenation, and coupling, on well-characterized single-crystal surfaces by providing molecular level insight into the bond breaking and formation on surfaces that are the basis for heterogeneously catalysis. The ultimate goal of such research is to provide benchmarks for theory, forming a firm basis for *a priori* catalyst design. In the nearer term it provides a kernel of information which can be combined with theory to accurately predict rates and selectivities for extended series of analogous reactions outside the data set. In this talk, these concepts will be discussed, linking fundamental surface science studies on Au single crystals with the performance of dilute Au-based dilute metal alloy catalysts operating at elevated temperature and 1 atm pressure. The use of key surface-science methods, including XPS, vibrational spectroscopy and temperature programmed reaction spectroscopy, will illustrate the methodology for understanding catalytic reactions. This work demonstrates the ability to successfully predict surface

[1] **Gaede Langmuir Award Winner**

reactivity across vast regimes of pressure, temperature and materials complexity.

Quantum Information Science Focus Topic
Room 302 - Session QS+EM+MN+NS-ThA

The Quantum Metrology Revolution

Moderator: Dave Pappas, Rigetti Computing

2:20pm **QS+EM+MN+NS-ThA-1 Magnetic Textures in Quantum Materials Revealed by SQUID-on-tip Microscopy**, ***Ella Lachman***, Rigetti Computing **INVITED**

Quantum materials are rapidly emerging as the basis for possible novel computation devices. However, fully understanding the interplay between magnetic and electronic excitations prevents us from realizing their full potential. In my talk, I will present the nano-SQUID-on-tip device and the scanning microscope built around it. Originally built to study superconducting vortex dynamics, this microscope has unprecedented magnetic sensitivity and spatial resolution.

I will show how expanding the microscope's range and realizing the microscopic magnetic textures in quantum materials is crucial to the understanding of transport phenomena on the macro scale. This will be demonstrated with two examples from two different types of materials. First, I will show how scanning nanoSQUID-on-tip magnetic imaging of magnetically doped topological insulators reveals the underlying fragility of the Quantum Anomalous Hall effect at elevated temperatures. Then, I will show how with a combination of transport, magnetization, and magnetic imaging of the Weyl semimetal $Co_3Sn_2S_2$, we find that the dynamics of domain walls are responsible for the anomalous transport behavior in the material.

These examples show that better understanding of the microscopic magnetism in these systems reveal new phenomena and deepen our understanding of the interplay between magnetic textures and electronic properties.

3:00pm **QS+EM+MN+NS-ThA-3 Quantum-Based Measurements for Pressure and Vacuum and the NIST on a Chip Program**, ***Jay Hendricks***, *B. Goldstein,* NIST

The world of pressure and vacuum measurements and standards is currently undergoing a revolution in both measurement traceability, “the fundamental philosophy behind a measurement chain back to primary units”, and measurement technology, the “how a measurement is made”.This keynote presentation covers a bit of metrology history of how we got to where we are today and gives a forward-looking vision for the future.The role of NIST as a National Metrology institute is described along with an explanation of how and why our world-wide standards changed on May 20th, 2019.The NIST on a Chip program (NOAC) is introduced which seeks to utilize fundamental physics and laws of nature to develop quantum-based sensors and standards that one day may be miniatured to the chip scale.The technical core of the lecture will be a deeper dive into new research on measurement methods for pressure, the Fixed Length Optical Cavity (FLOC) and for vacuum, the Cold Atom Vacuum Standard (CAVS).What is exciting about these new measurement approaches is that they are both primary (relying on fundamental physics), are quantum-based and use photons for the measurement readout which is key for taking advantage of the fast-growing field of photonics. The FLOC will enable the elimination of mercury barometers pressure standards worldwide and the CAVS will be first primary standard for making vacuum measurements below 1.3x10-5 Pa.

3:20pm **QS+EM+MN+NS-ThA-4 Materials and Devices for Efficient Quantum Memories and Sensors**, ***Lee Bassett***, University of Pennsylvania **INVITED**

Certain point defects in semiconductors exhibit quantum-mechanical features comparable to isolated atoms or molecules, in a solid-state materials platform amenable to nanofabrication, heterointegration with other materials and classical devices, and large-scale system engineering. Well-known quantum point defects such as the diamond nitrogen-vacancy center are leading candidates as robust quantum memories, versatile quantum sensors, and efficient light-matter interfaces. Meanwhile it is increasingly clear that alternative materials and defect systems offer potential advantages and new capabilities for quantum science [1]. However, millions of potential defects exist, and their identification is often tedious and challenging. This talk will introduce the opportunities and challenges of identifying point defects, including several new approaches to efficiently predict, characterize, and engineer their properties for quantum science and technology.

[1] L. C. Bassett, A. Alkauskas, A. L. Exarhos, and K.-M. C. Fu, "Quantum defects by design" Nanophotonics 8, 1867 (2019).

Funding: We acknowledge support from the NSF (DMR-1922278 and DMR-2019444).

Electronic Materials and Photonics Division
Room 304 - Session EM1+MN+NS-FrM

Piezoelectric, Ferroelectric, and Multiferroic Devices & Microelectronics

Moderators: M. David Henry, Sandia National Labs, **Stephen McDonnell**, University of Virginia

8:20am **EM1+MN+NS-FrM-1 Piezoelectric Adjustable X-ray Optics*, Susan Trolier-McKinstry,*** Penn State University **INVITED**

Next generation X-ray observatories require lightweight, high throughput optics that maintain a < 0.5 arcsecond resolution. Thin adjustable X-ray mirrors can correct deformations generated from fabrication errors, gravity release, mounting stresses, and thermal variations, maintaining the high angular resolution (< 0.5 arcsecond) and large effective area (> 2 m^2) required for future X-ray missions. This paper describes fabrication of adjustable mirrors for the Lynx X-ray observatory mission concept.Prototype X-ray mirrors were built on either a 400 µm thick curved *Corning EAGLE XG®*glass substrate or on polished Si.In both cases, a Cr/Ir X-ray mirror coating was deposited on the front (concave) side, and an array of 1.5 µm thick radio frequency (RF) sputtered $Pb_{0.995}(Zr_{0.52}Ti_{0.48})_{0.99}Nb_{0.01}O_3$(PZT) piezoelectric thin film actuators on the back (convex) side to enable correction of figure errors.A two-layer metal routing scheme with a polymeric insulator was used to independently address 288 actuators on the mirror. The two-layer metal allows narrow kerfs between actuators and increased actuator density. A chrome-iridium layer was deposited on the concave side to function as the X-ray reflective coating for the films deposited on the convex side.Anisotropic conductive film was used to bond thin flexible copper cables to flat edges of the mirror to interface with external control electronics. Improved stress balancing process was achieved using compressively stressed SiO_2 films deposited on the convex side of the mirror to balance the tensile integrated stress of the actuator array while also matching the film thickness distribution.Finite element methods were used to assess the impact of film thickness distributions on the convex and concave substrate surfaces.The resulting models show peak-to-valley figure errors of 105 nm, well within the 1 µm peak-to-valley dynamic range of the piezoelectric adjusters. In contrast, when stress compensation was done with an iridium mirror film deposited on the front side, the mismatched thickness distribution results in peak-to-valley figure errors over 3 µm.

9:00am **EM1+MN+NS-FrM-3 Oxide and Nitride Ferroelectric Wurtzite Crystals*, Jon-Paul Maria,*** Penn State University

In the past three years, the demonstration of ferroelectricity in wurtzite-based crystals introduced exciting opportunities to explore and discover new structure-property relationships in novel formulation spaces, and to investigate new integration and device implementations given new process compatibilities. The seminal discovery of ferroelectric $Al_{1-x}Sc_xN$ by Fichtner *et al.* initiated this excitement and was followed by comparable observations of polarization reversal in the structurally similar $Al_{1-x}B_xN$[2] and the $Zn_{1-x}Mg_xO$[3] systems.

In this presentation our group will present recent results that demonstrate the structure-process-property relationships in the B-substituted AlN and Mg-substituted ZnO nitride and oxide systems. The B-substituted materials exhibit square hysteresis loops with polarization values between 150 µC/cm^2 and 120 µC/cm^2 when boron concentrations range between 2% and 15% respectively. Coercive field values fall with additional boron, from 5.5MV/cm to about 5 MV/cm at B saturation. Bandgap values are approximately 5 eV or above in all cases. Material can be prepared between 100 °C and 350 °C with very little difference in electrical properties. W bottom and top electrodes are used in all cases. Capacitors can be prepared down to 50 nm thick before leakage current becomes problematic during low frequency hysteresis measurements. First principles calculations that rationalize the unit cell volume, bond angle distribution, and remanent polarization will be presented.

Comparable results are found in the $Zn_{1-x}Mg_xO$ system. Between 25% and 35% Mg substitution, square hysteresis loops with remanent polarization values above 100 µC/cm^2 are readily achieved. Transmission measurements show bandgap values between 4.0 eV and 4.2 eV in this range. In comparison to AlBN, coercive field values for ZMO are as low as 1.7 MV/cm. As is the case with AlBN and AlScN, sustaining high insulation resistance to arbitrarily low thickness is challenging, the current thinness limit for low-leakage switching is ~ 125 nm. SHG analysis will also be presented for the ZMO system – preliminary measurements suggest values comparable to ferroelectric niobates.

9:20am **EM1+MN+NS-FrM-4 Development and Processing of $Al_{1-x}Sc_xN$ (x<0.40) Films for Resonator and Filter Applications*, Giovanni Esteves,*** *S. Yen, T. Young,* Sandia National Laboratories*; Z. Tang,* The University of Pennsylvania*; E. Schmidt, L. Gastian, M. Henry, T. Bauer, C. Nordquist,* Sandia National Laboratories*; R. Olsson,* The University of Pennsylvania

As the development of aluminum scandium nitride ($Al_{1-x}Sc_xN$/AlScN) films continues to be pushed towards higher Sc content, fabricated devices yield insight into the challenges associated with processing while demonstrating increased electromechanical coupling coefficients (k_t^2) over AlN. The addition of Sc into AlN presents film development and fabrication challenges that increase with higher Sc content such as the reduction of abnormal grains (AG), higher compressive stress, and etching. The development of $Al_{0.6}Sc_{0.4}N$ films using a single-alloyed target poses a significant challenge in terms of managing stress and the density of AG. Compressive stress help in reducing the amount of AG density through tuning the Ar/N_2 flow and pressure, but the magnitude of stress needed to achieve a low density of AG exceed -600 MPa. The use of certain metal templates aid in reducing AG density but are not sufficient to achieve AG-free films. Etching AlScN leads to long etch times due to slow etch rates of 25 nm/min and result in sidewall angles of ~74°. Nevertheless, AlScN lamb wave resonators (LWR) have been fabricated to demonstrate k_t^2 over 10%. Additionally, LWR with varying k_t^2 were interconnected to fabricate ladder filter configurations to determine that amount of bandwidth increase that can be achieved over AlN. Though AlScN demonstrates higher k_t^2, that lead to higher bandwidth, pushing this current technology to achieve more desirable metrics requires more stringent process quality.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

9:40am **EM1+MN+NS-FrM-5 Formation of Aluminum Scandium Nitride Microelectromechanical Systems Via Etching in Aqueous Potassium Hydroxide (KOH)*, Zichen Tang,*** *M. D'Agati, R. Beaucejour, S. Sofronici, J. Zheng, K. Kaylan,* University of Pennsylvania*; G. Esteves,* Sandia National Laboratories*; R. Olsson,* University of Pennsylvania

We report on the etch rate of sputter deposited piezoelectric and ferroelectric Aluminum Scandium Nitride ($Al_{1-x}Sc_xN$) thin films in aqueous potassium hydroxide (KOH). Specifically, we report on the vertical etch rate, lateral etch rate, and sidewall angle as a function of the scandium alloying ratio (x), temperature, and KOH concentration. As the scandium alloying ratio is increased, the vertical etch rate in 30% KOH at 45 °C is reduced from > 100 nm/s for AlN to < 4 nm/s for $Al_{64}Sc_{36}N$. The lateral etch rate, however, follows a very different trend, arriving at a minimum values of 0.05 nm/sec for $Al_{88}Sc_{12}N$. This is in contrast to the much higher lateral etch rates observed for both AlN and $Al_{64}Sc_{36}N$ of 2 nm/s. These trends in vertical and lateral etch rate are shown to hold for KOH concentrations from 10 to 30% and etch temperatures from 45 to 65 °C. We show that the etched sidewall angle can be predicted from a combination of the crystal structure and the vertical and lateral etch rates. We report a technique that utilizes the crystal structure and the vertical and lateral etch rates to form vertical (i.e. 90°) sidewalls solely from aqueous KOH etching. The ability to control the sidewall angle is vitally important in the formation of microelectromechanical systems (MEMS). We report on several piezoelectric MEMS devices fabricated utilizing the KOH etching processes. Finally, we report on the etching of AlScN as a function of ferroelectric polarization.

10:00am **EM1+MN+NS-FrM-6 Interface Reactions During the Ferroelectric Switching of HfZrO Thin Films on InAs*, A. Irish, Y. Liu, R. Atle, A. Persson, R. Yadav, M. Borg, L. Wernersson, Rainer Timm,*** Lund University, Sweden

Traditional MOSFET-based electronic components have reached severe bottlenecks regarding data handling speed and power dissipation. A very promising alternative approach builds on MOS material stacks with thin ferroelectric oxide films in novel device architectures for e.g. steep-slope transistors, neuromorphic networks, or in-memory computation [1]. $Hf_{1-x}Zr_xO_2$ (HZO) films grown by atomic layer deposition are widely used in this context, due to their excellent film quality and conformity with existing semiconductor technology. Ferroelectric MOS devices based on III-V semiconductors are especially promising for high-speed applications due to the high charge carrier mobility of e.g. InAs. Furthermore, InAs/HZO/TiN devices have shown an unexpectedly high remanent polarization of the ferroelectric film [2]. In spite of the excellent electrical performance, only little is known about the structure, chemical composition, and switching dynamics of the semiconductor-ferroelectric oxide interface. We have

previously used X-ray photoemission spectroscopy (XPS) to investigate interfaces of ferroelectric HZO [3], but *in situ* structural characterization obtained during the ferroelectric switching has been lacking until now.

Here, we present operando hard X-ray photoelectron spectroscopy (HAXPES) results from ferroelectric InAs/HZO/TiN MOS devices obtained during electrical biasing and switching. We observe an interface layer consisting of In- and As-oxides at the InAs/HZO interface. As 2p and In 3d core level spectra were obtained after subsequent switching processes of a "positive-up-negative-down" (PUND) series, showing a reproducible increase of the amount of interface oxide upon upward polarization and a decrease upon downward polarization. Thereby, electrical PUND cycles confirm the ferroelectric nature of the MOS device. Such a redox reaction at the semiconductor-oxide interface upon ferroelectric switching has – to our knowledge – not been reported before. Furthermore, we observe that the major fraction of the applied bias does not drop over the 10 nm thin HZO layer, but instead over the thin InAs-oxide interface layer.

These observations are challenging the established understanding of ferroelectric behavior in thin oxide films and are a key to understanding the superior performance of III-V/HZO based devices.

[1] M. Park et al., MRS Commun. **8,** 795 (2018).
[2] A. Persson et al., Appl. Phys. Lett. **116**, 062902 (2020).
[3] R. Athle et al., ACS Appl. Mat. Int. **13**, 11089 (2021).

10:20am **EM1+MN+NS-FrM-7 The Effect of Hf Doping on Piezomagnetic Properties of FeCo for Magnetoelectric Heterostructure Devices***, **Thomas Mion**, K. Bussmann, M. Staruch, P. Finkel,* US Naval Research Laboratory

New developments in magnetoelectric devices have demonstrated increased energy efficiency and temperature stability with reduced size compared to current technologies. Artificial magnetoelectrics, built on the combination of ferromagnetic magnetostrictive materials structurally coupled to piezoelectric and ferroelectric materials, display the ability to control magnetic properties of the ferromagnet with electric voltage across the piezo/ferroelectric layer. The best performance requires the implementation of soft magnetic materials with large magnetostriction and large voltage-induced strain in the piezo/ferroelectric layer. Processing requirements for device fabrication often complicate the realization of these combined qualities as inherent stresses from the deposition technique are often detrimental to the magnetoelectric functionality. Solutions to these problems are rarely reported though alloying of FeCo and subsequent metalloid substitutions such as $(Fe_{0.5}Co_{0.5})_{1-x}C_x$, and $(Fe_{0.5}Co_{0.5})_{1-x}B_x$, have proven successful in reducing the coercive field while retaining high magnetostriction and piezomagnetic properties **[1,2]**.

In this work we present the systematic study of sputter-deposited Hf-doped $Fe_{50}Co_{50}$ alloy thin films with a focus on the correlation between film stress and magnetic softness and find an inflection point from tensile to compressive stress with increasing Hf composition. Scanning electron microscopy (SEM) and X-ray diffraction (XRD) of the $(Fe_{0.5}Co_{0.5})_{1-x}Hf_x$ system reveal the magnetic softening is also correlated to emergence of an amorphous phase with reduced grain size for these sputter-deposited films. We will show the utilization of this new alloy in a multiferroic MEMS resonator device demonstrating a high magnetoelectric response required for magnetic sensors.

[1] Phys. Rev. Applied 12, 034011 (2019)

[2] Appl. Phys. Lett. 91, 182504 (2007)

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