2D Materials Focus Topic
Room 201B - Session 2D+EM+MI+NS+TF-MoM

2D Materials Growth and Fabrication

Moderator: Jing Xia, University of California Irvine

8:20am **2D+EM+MI+NS+TF-MoM1 Wafer Scale Epitaxial Growth of Monolayer and Few-Layer WS_2 by Gas Source Chemical Vapor Deposition**, ***Mikhail Chubarov***, *T.H. Choudhury, J.M. Redwing,* The Pennsylvania State University

Tungsten disulfide (WS_2) has been widely investigated due to its outstanding properties compared to other 2D TMD including a bandgap of 2 eV, relatively high theoretical electron mobility, valley spin polarization, among others. Commonly, the films are grown on amorphous substrates like SiO_2 and, consequently, consist of high angle grain boundaries after coalescence due to the random orientation of domains. These can act as scattering and recombination centers for charge carriers limiting device performance. To avoid this, a crystalline substrate and epitaxial growth is typically employed for general thin film deposition although this approach has not been extensively investigated for 2D TMD monolayers. Large area growth is also crucial to show technological feasibility of the material for wafer-scale device fabrication.

In this work, we employ cold wall gas source chemical vapor deposition for the growth of WS_2 films on 2" (0001) α-Al_2O_3. To achieve coalesced monolayer growth over the entire substrate, we implemented a multi-step growth process modulating the metal precursor concentration during each of the steps. $W(CO)_6$ and H_2S were used as precursors in H_2 carrier gas. The deposition experiments were conducted over the temperature range from 750 °C to 1000 °C at a pressure of 50 Torr. Characterization of resulting samples was conducted using atomic force microscopy (AFM), in-plane X-ray diffraction (XRD) and room temperature Raman and photoluminescence (PL) measurements.

Initial studies showed that the WS_2 films exhibit multiple crystal orientations which evolve with growth temperature. At lower deposition temperature (750 °C), two orientations rotated 30° one from another were observed. At the high deposition temperature (1000 °C), five different crystal orientations were present. Among others, orientation with epitaxial relation of (10-10)WS_2//(10-10)α-Al_2O_3 was present at all temperatures. It was established that the unwanted orientations can be suppressed by increasing the H_2S concentration. Further adjustment of the growth and use of the multi-step growth process led to the formation of a coalesced epitaxial monolayer WS_2 on α-Al_2O_3 with XRD FWHM of 10-10 peak in ω being 0.09°. This value suggests well in-plane oriented domains with low edge dislocation density. A high intensity, narrow (FWHM=40 meV) PL peak positioned at 2.01 eV was observed for WS_2 films. Monolayer formation was confirmed from the AFM height profile (D =0.9 nm) and Raman measurements by observing spectral region where layer breathing and shear modes would appear. A fully coalesced, monolayer film was achieved using the multi-step growth process in a total time of 80 minutes.

8:40am **2D+EM+MI+NS+TF-MoM2 Wafer Scale Deposition of Monolayer Transition Metal Dichalcogenides**, ***Kortney Almeida***, *M. Wurch, G. Stecklein, L. Bartels,* University of California, Riverside

Monolayer transition metal dichalcogenide (TMD) films are promising materials in the continuing development of nanoscale devices. Methods to produce wafer-scale monolayer TMD films have included tube-furnace chemical vapor deposition (CVD), liquid-phase exfoliation, and metal-organic CVD. These methods suffer from issues with particulate contamination, pyrophoric precursors, and high cost. Here we demonstrate the growth of homogeneous wafer-scale monolayer molybdenum disulfide (MoS_2) using solid inorganic and liquid organic precursors in a high-vacuum environment. These results are achieved using an amorphous SiO_2substrate and without any powder or metal-organic precursors. Growth proceeds by the decomposition of carbon disulfide at a hot molybdenum filament, which yields volatile MoS_xprecursors that precipitate onto a heated wafer. The continuous and homogeneous single-layer film of $MoS_2$is deposited at wafer scale with a total growth time of fifty minutes. Various thicknesses of the thin films are also demonstrated by the manipulation of the filament power. Optical and electrical characterization indicates performance comparable to or better than MoS_2film grown by other wafer-scale growth techniques. Our method provides a scalable process to deposit thin TMD films in a high vacuum environment.

9:00am **2D+EM+MI+NS+TF-MoM3 Crystal Growth of 2D Materials: From Model Systems to Integrated Manufacturing**, ***Stephan Hofmann***, University of Cambridge, UK **INVITED**

In order to serve the industrial demand for "electronic-grade" 2D materials, we focus on chemical vapour deposition (CVD), and in this talk I will review our recent progress in scalable CVD [1] and device integration approaches of highly crystalline graphene, hexagonal boron nitride (h-BN) and transition metal dichalcogenide films. The systematic use of in-situ metrology, ranging from high-pressure XPS to environmental electron microscopy, allows us to reveal some of the key growth mechanisms for these 2D materials that dictate crystal phase, micro-structure, defects, and heterogeneous integration control at industrially relevant conditions [2,3]. I will focus on tailored CVD processes to achieve large monolayer h-BN domains with lateral sizes exceeding 0.5 mm. Importantly we show that depending on the process catalyst as-grown h-BN mono-layers can be easily and cleanly transferred using an entirely exfoliation-based approach.[4] We demonstrate sequential h-BN pick-up, opening a pathway to integrate CVD films in high quality 2D material heterostructures. Progress in growth reached a level where adequate characterisation of such 2D crystal layers over large areas has become a key challenge. Hence we also explore new non-contact characterisation methods [5,6]. We work on applications ranging from magentic tunnel junctions [7] to sensing and single molecule analysis [8,9], and the talk will focus on some of the diverse yet connected integration challenges for CVD 2D films that present a key bottleneck towards reliable scale-up manufacturing and commercialisation.

References

1. Hofmann et al., J. Phys. Chem. Lett. 6, 2714 (2015).

2. Weatherup et al., Nano Lett. 16, 6196 (2016).

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4. Wang et al., in progress (2018).

5. Lin et al., Sci. Rep. 7, 10625 (2017).

6. Feng et al., Nano Lett. 18, 1739 (2018).

7. Piquemal-Banci et al., ACS Nano (2018).

8. Dahmke et al., ACS Nano 11, 11108 (2017).

9. Walker et al., ACS Nano 11, 1340 (2017).

9:40am **2D+EM+MI+NS+TF-MoM5 Understanding the Edge-Controlled Growth and Etching in Two-Dimensional Materials**, ***Kai Xiao***, *X. Li, X. Sang,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; W. Zhao, J. Dong,* Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS), Ulsan,44919, South Korea*; A. Purektzy,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; C. Rouleau,* Center for Functional Nanomaterials Brookhaven National Laboratory*; F. Ding,* Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS), Ulsan,44919, South Korea*; R.R. Unocic, D.B. Geohegan,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Understanding the atomistic mechanisms governing the growth and etching of two-dimensional (2D) materials is of great importance in guiding the synthesis of large area, single-crystalline, high quality 2D crystals and heterostructures. In this talk, the growth-etching-regrowth process of monolayer 2D crystals by a CVD method will be discussed. We found that switching from growth to etching formed pores with various shapes in the single crystal domains which can be explained by edge-structure dependent growth process. In addition, combined with first principles theory, and ab initio simulations, in situ STEM imaging was used to understand the evolution of edge structure around pores in monolayers as a function of temperature and Mo chemical potential. Our results demonstrate that by varying the local chemical environment, we can trigger formation of 2D monolayer nanostructures terminated by different edge reconstructions during in situ heating and electron beam irradiation and form edge structures with metallic and/or magnetic properties. The ability to synthesize 2D nanostructures with metastable NW edges having predictable atomic structures opens the door to a wide range of novel 2D materials and heterosturctures with electrical and magnetic properties as revealed by DFT, which could potentially act as functional building blocks for next-generation nano-devices.

References:

[1] X. Li, J. Dong, J. C. Idrobo, A. A. Puretzky, C. M. Rouleau, D. B. Geohegan, F. Ding, K. Xiao, J. Am. Chem. Soc. 139, 482 (2017).

[2] X. Sang, X. Li, W. Zhao, J. Dong, C. M. Rouleau, D. B. Geohegan, F. Ding, K. Xiao, R. R. Unocic, Nature Comm. Accepted (2018).

Acknowledgement: Synthesis science sponsored by the Materials Science and Engineering Division, Office of Basic Energy Sciences, U.S. Department of Energy. Characterization science performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Sciences User Facility.

10:00am **2D+EM+MI+NS+TF-MoM6 Synthesis and Characterization of 1T, 1T', and 2H $MoTe_2$ Thin Films**, ***Thomas Empante,*** University of California, Riverside*; Y. Zhou,* Stanford University*; S.A. Naghibi Alvillar,* El Camino College*; E.J. Reed,* Stanford University*; L. Bartels,* University of California, Riverside

Transition metal dichalcogenides (TMDs) have been of interest over the past few decades for their intriguing structural, electronic, and optoelectronic properties, particularly when scaled down to thin films. One of the most interesting TMD materials is molybdenum ditelluride ($MoTe_2$) because of its relative ease to attain multiple phases at room temperature, namely the metallic 1T' phase and the semiconducting 2H phase. Here we show a facile chemical vapor deposition process to synthesis not only the aforementioned phases but the elusive unreconstructed 1T phase by regulating the cooling rate and the addition of carbon dioxide during the reaction. Our experimental Raman spectroscopy results were compared to theoretical density functional theory calculations which verify the synthesis of all three phases. Electronic transport measurements were also used to characterize the films and show that the newly synthesized 1T phase is in good agreement with theoretical models depicting semi-metallicity as the material shows increased conductivity with elevated temperatures. In addition to the pure phase materials, mixed phase materials, such as 2H/1T, can be synthesized with slight alterations to the parameters leading to enhancements of the 2H phases' conductivity.

11:20am **2D+EM+MI+NS+TF-MoM10 Low-Defect, High-Uniformity Transfer-Free Graphene on SiO_2 by Thermal Chemical Vapor Deposition**, ***Leslie Chan,*** *D.S. Tsai, Z. Wang, C. Carraro, R. Maboudian,* University of California, Berkeley

Chemical vapor deposition (CVD) has emerged as the customary approach for scalable, controllable production of graphene for integrated devices. Standard CVD graphene must be transferred from a generic metal growth substrate onto the desired substrate (*e.g.*, SiO_2), but this extra transfer often leads to wrinkles, contamination, and breakage that ultimately result in poor device performance. Several groups have demonstrated metal-catalyzed direct CVD-graphene growth on insulating substrates, but the final graphene products are deficient in quality and uniformity. This work details an expansion of the parameter space that enables lower-defect, higher-uniformity graphene than previously reported using nickel and copper catalysts, respectively. We introduce a mechanism based on carbon permeability that provides deeper insight into the growth process. Ultimately, these studies seek to inform the judicious choice of process parameters that will lead to large-area, high-quality, layer-controlled graphene directly on target substrates.

Nanometer-scale Science and Technology Division

Room 102B - Session NS+2D+AN+EM+MN+MP+PC+RM-MoM

IoT Session: Nanostructured Devices and Sensors

Moderators: David Czaplewski, Argonne National Laboratory, Liya Yu, NIST Center for Nanoscale Science and Technology

8:20am **NS+2D+AN+EM+MN+MP+PC+RM-MoM1 Integrating Nanodiamonds with Augmented Artificial Intelligence and Digital Health to Optimize Combination Therapy**, ***Dean Ho,*** UCLA **INVITED**

Dean Ho, Ph.D.

Nanodiamonds have emerged as promising candidates for clinical drug delivery due to their ability to carry a wide range of candidate therapies, unique surface properties, and biological tolerability. This lecture will highlight our recent clinical trial to validate a nanodiamond-embedded biomaterial for root canal therapy indications [1]. We will discuss the broad spectrum of efficacy, safety, characterization, and other studies that bridged in vitro with preclinical and downstream in-human studies. This lecture will also discuss upcoming clinical nanodiamond-based drug carrier studies, as well as our work in augmented artificial intelligence (AI) to develop globally optimized nanodiamond-modified therapy. Pairing nanodiamond platforms with augmented AI will lead to major advances in drug development and markedly improve response rates and treatment outcomes for a broad spectrum of disorders. Our recent clinical trials using these powerful combination therapy optimization technologies and digital health platforms to scale their implementation to usher in a new era of nanomedicine-based treatment will also be discussed [2].

1. Lee et al., Proceedings of the National Academy of Sciences, 2017

2. Zarrinpar et al., Science Translational Medicine, 2016

9:00am **NS+2D+AN+EM+MN+MP+PC+RM-MoM3 Morphology-Controlled Large-Scale Tin Oxide Nanostructures for Highly Sensitive Room Temperature Gas Sensor**, ***Amrit Sharma,*** Norfolk State University

Highly sensitive large-scale tin oxide (SnO_2) nanostructures were grown on a glass substrate by vapor-liquid-solid (VLS) process using a mixture of anhydrous tin (II) chloride ($SnCl_2$) and zinc chloride ($ZnCl_2$) powders. We demonstrate a new kind of single cell vapor deposition system to precisely control nanostructural morphology by changing the weight ratio of $SnCl_2$ and $ZnCl_2$ and growth temperature. The morphology and structural property of as-grown nanostructures were characterized using scanning electron microscopy (SEM) and X-ray diffraction (XRD). The SEM images revealed that the SnO_2 nanostructures with different densities, sizes, and shapes can be achieved by adjusting the weight ratio of $SnCl_2$ and $ZnCl_2$. SnO_2 nanostructures with diameter ~20 nm and length ~100 nm showed ~85% sensitivity and 53 seconds of response time, whereas the nanorods with diameter ~100 nm and length ~ 1mm showed ~50% sensitivity with 198 seconds response time. The nanostructured material with small size and shape showed better sensitivity on sensing at room temperature compared to previously reported SnO_2 based sensors.

9:20am **NS+2D+AN+EM+MN+MP+PC+RM-MoM4 Improving the Localized Surface Plasmonic Resonance Sensing Properties by Composite Metal/Dielectric Mixtures**, ***Steven Larson***[1], *Y. Zhao,* University of Georgia

Localized surface plasmon resonance (LSPR)-based sensors, whose resonance absorbance wavelength responds to the change in the local dielectric environment have attracted great attention and have been widely studied over the past decade. These sensors are traditionally improved by modifying the shape, size, and gap in the plasmonic nanostructure of the sensor. The sensitivity can also be tuned by the dielectric constant of the plasmonic material, such as noble metal alloys, but the improvements are not significant. Here we show that using a metal-dielectric composite, one can significantly improve the sensitivity of a LSPR sensor. Regular nanotriangle pattern samples composed of a mixture of Ag and MgF_2 with different composition ratios are prepared by combining nanosphere lithography and electron beam co-deposition. The plasmon resonance of these composite nanostructures at high Ag composition (C_{Ag})are shown to redshift with C_{Ag} until a composition threshold ($C_{Ag} \leq 90\%$) is met, where the resonance wavelength is nearly constant, slightly blue shifting. Multiple morphological and compositional characterization techniques are used to confirm that the shifts in the plasmonic properties are due to the change in composition and not a change in the morphology. The resulting LSPR sensor at C_{Ag} = 90 at.% can achieve a sensitivity of 696 RIU/nm, as compared to 312 RIU/nm for the same nanotriangle with pure Ag. This significantly improved sensitivity is due to the modified dispersion relationship of the dielectric constant by the composite and will play an important role in future plasmonic material design and applications.

9:40am **NS+2D+AN+EM+MN+MP+PC+RM-MoM5 Improving the Selectivity of Tin (IV) Oxide Paper Based Gas Sensors with Plasma Surface Modification**, ***Kimberly Hiyoto,*** *E.R. Fisher,* Colorado State University

Metal oxide nanomaterials are desirable for solid-state gas sensors because of their ability to detect a wide variety of gases through changes in resistance resulting from gas-surface interactions. When optimizing these sensors, the supporting substrate is rarely considered, resulting in devices that are often brittle and have a fixed amount of nanomaterial that can be exposed to target analytes. Recent work using paper as the supporting substrate yields more affordable sensors that are flexible, allowing for a more robust device. Furthermore, the porous morphology of the paper also provides a larger surface area to attach metal oxides when compared to a traditional flat substrate of the same dimensions. Another limitation of these metal oxide sensors is inherent in the detection method. The lack of selectivity and required operating temperature of ≥300 °C limits the widespread use of metal oxide sensors. Dopants or the addition of a filter in the device design are typical approaches to address these problems;

[1] **NSTD Student Award Finalist**

however, this increases fabrication complexity and cost. Plasma processing is a promising strategy to address these issues because it maintains desirable bulk properties but modifies the surface of the material to enhance gas sensor performance.

Here, we describe the Ar/O_2 plasma modification of paper based, tin (IV) oxide (SnO_2) nanoparticle devices as a function of applied rf power and precursor pressure. After plasma modification, the paper-based sensors exhibited improved response to carbon dioxide, ethanol, and benzene when compared to the untreated material on a more traditional substrate, zirconium dioxide. Additionally, sensor response to a target gas changed depending on the plasma modification parameters used, indicating the selectivity of these SnO_2 sensors can be easily tailored via plasma processing. Response and recovery studies of both the treated and untreated sensors will be discussed to demonstrate the dynamic behavior of these devices to the target gases as another measure of gas sensor performance and durability. Along with sensing behavior, optical emission spectroscopy and X-ray photoelectron spectroscopy provide insight into how the plasma modified the material, ultimately elucidating the relationship between material surface chemistry and sensor selectivity. Finally, preliminary work using this same fabrication process with another type of metal oxide gas sensor will be discussed to demonstrate the applicability of this method for other types of materials. Ultimately, these data work toward improved understanding of the gas sensing mechanism to design better performing gas sensors.

10:00am **NS+2D+AN+EM+MN+MP+PC+RM-MoM6 TiN@Si_3N_4 Core-shell Heterostructures as Nanoantennas for Photocatalytic Reforming of Methanol**, ***Alejandro Alvarez Barragan***, *L. Mangolini,* University of California, Riverside

The light-harvesting capacity of plasmonic nanoparticles has recently garnered attention in the synthesis of nanoantennas for photocatalysis. Aluminum, gold, and silver have been used to successfully drive hydrogen dissociation and CO oxidation reactions by injecting hot electrons into chemically active catalysts —such as platinum and palladium— adsorbed to their surface. However, the low response of aluminum at visible-near infrared (vis-NIR) wavelengths, the high cost of silver and gold, and the low thermal stability of these three metals, inspire the quest for alternative plasmonic materials that could potentially expand the field towards more ambitious and cost-effective applications. Titanium nitride (TiN) is a conductive ceramic with high hardness and bulk melting point (2930 °C). Its plasmon resonance located in the vis-NIR region, low cost relative to gold and silver, and well-understood properties as a thin film in the semiconductor industry, make it a strong alternative to mainstream plasmonic metals. The present work encompasses a comprehensive study of the oxidation kinetics of TiN particles at the nanoscale and an exploration of its role as nanoantennas for light-induced methanol reformation. TiN particles are synthesized via a scalable, modular, non-thermal plasma method. Titanium and nitrogen precursors are transported into a RF frequency plasma where TiN particles nucleate and grow. The high surface area and nitrogen deficiency of the particles facilitate the oxidation of the material and weaken its plasmonic response. The introduction of a secondary reactor with an input of SiH_4 as precursor gas leads to the formation of a Si_3N_4 coating. STEM and XPS analyses show that Si_3N_4 acts as a diffusion barrier, dramatically reducing the oxidation of the ~8 nm TiN particles. UV-vis-NIR spectrophotometry data show that the core-shell heterostructures experience a substantial blue-shift of the plasmon peak and an increase in intensity compared to the bare TiN. Platinum nanoparticles were subsequently deposited on the TiN@Si_3N_4 by photo-induced reduction of an aqueous solution of chlorplatinic acid. After rinsing and centrifuging, the Pt/TiN@Si_3N_4 heterostructures were diluted in a 50:50 water/methanol solution. Upon photoexcitation via white light illumination, hydrogen generation was readily detected by gas chromatography. This work also highlights the wide range of applications available for light-induced processes, ranging from materials processing (deposition of Pt particles) to photocatalysis (methanol reforming). It also strengthens the case for alternative plasmonic materials in a field dominated by precious metals.

10:40am **NS+2D+AN+EM+MN+MP+PC+RM-MoM8 Nanostructured Sensor and Device Applications of Infiltrated Zinc Oxide**, ***Leonidas Ocola***, Argonne National Laboratory; *Y. Wang, J. Chen,* University of Wisconsin-Milwaukee; *P. Blaisdell-Pijuan,* California State University-Fullerton; *R. Divan,* Argonne National Laboratory **INVITED**

With the increased portfolio of materials deposited using atomic layer deposition (ALD) there has been an increased interest in infiltrated metal oxides such as zinc oxide for novel applications. We find that ZnO metal oxide ALD infiltration can be useful for nanoscale resolution imaging of biological samples and to fabricate novel UV and gas nanosensors with high sensitivity. The ALD infiltration utilizes similar concepts of the ALD coating process with the significant difference in process exposure times, pressure, and purpose. The purpose is to allow the precursor gases infiltrate a porous media (such as a dry biological sample or a photoresist polymer) and allow the reaction to occur inside the material matrix.

In terms of device fabrication we use SU8 as a negative resist that allows for localization of the infiltration process. We have used this property to make a device that is UV sensitive, and that is sensitive to ppm concentrations of gases by using infiltrated zinc oxide. The large bandgap and semiconductor properties of ZnO allow for a visible-blind ultra violet light sensor. We used a standard UV flashlight that emits at 408 nm as the UV source. We also tested the same device for sensing gases like nitrous oxide and formaldehyde. We show that the device can detect these gases with concentrations of 5 ppm. The change in current for such low concentrations was measured to be between 25% and 35 %.

With the purpose of investigating quantum applications of infiltrated ZnO, we also have characterized the growth of ZnO in PS-b-PMMA block copolymers (BCP) of spherical and cylindrical sub-20 nm morphologies and studied how the photoluminescence of these nanostructures varies per its seed layer. We report blue-shifted photoemission at 335nm (3.70eV), suggesting quantum confinement effects. Samples of ZnO prepared with an alumina seed layer showed additional defect state photoemission at 470nm and 520nm for spherical and cylindrical BCP morphologies, respectively. Defect photoemission was not observed in samples prepared without a seed layer. No Raman peaks were observed for any samples with less than four cycles of ZnO, implying the absence of phonons and the functionality of these ZnO nanostructures as isolated emitters. To that effect we have demonstrated a fabrication path to isolate single infiltrated cylinders, paving the way for further studies of optical properties of individual 20 nm ZnO nanostructures.

- Use of the Center for Nanoscale Materials an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

11:20am **NS+2D+AN+EM+MN+MP+PC+RM-MoM10 Templates for the Investigation of Size-Selected Nanocluster Networks**, ***Patrick Edwards***, *V.V. Kresin,* University of Southern California

The study of metal nanoclusters has revealed quantum nanoscale effects unique to the fully size-resolved regime. A highly notable example is electronic shell structure, akin to that in atoms and nuclei, which arises when confined conduction electrons organize into discrete energy levels. One consequence is the possibility of dramatic enhancement in electron Cooper pairing. Recent research from our group has provided evidence of this enhancement in certain free Al nanoclusters, with the electronic transition taking place at a temperature two orders of magnitude above that of bulk aluminum. We now aim to take advantage of this phenomenon by exploring the pairing transition in size-selected nanoclusters soft-landed on an appropriate substrate. Of particular interest are graphene and nanotube device architectures which provide unique templates for organizing nanocluster arrays. For example, a network of such superconducting nanoislands may induce superconductivity in graphene even at low coverages. Theory also predicts that an array of nanoclusters will not only support, but even enhance the Josephson current by 2-3 orders of magnitude. Carbon allotropes offer two distinct advantages for our system. First, the weak out-of-plane bonding provides a surface with less potential to disturb the structure of the soft-landed nanoclusters. Second, the tunability of graphene and carbon nanotube-based field effect transistors offers a versatile probe of nanocluster properties. We are also investigating the use of biological nanowires (bacterial flagella) as potential scaffolds upon which to deposit such nanocluster networks. These abundant and naturally occurring nanowires could serve as low cost and highly reproducible alternatives to the more common metallic or semiconductor templates.

Research supported by the Army Research Office (W911NF-17-1-0154).

11:40am **NS+2D+AN+EM+MN+MP+PC+RM-MoM11 High Performance Detection for X-ray and g -ray with $MAPbX_3$ Perovskite Single Crystals**, *X. Wang, Z. Zhu, Q. Li, J. Wu, X. Zhang, B. Wang,* ***Wei Lei***, Southeast University

Recently, organometallic lead trihalide perovskites have emerged as a new generation of opto-electronic materials. However, the high performance detection for x-ray and gamma-ray with $MAPbX_3$ is still a big challenge. For x-ray and gamma-ray detections, the detectors should have high sensitivity.

If the photon counting method is adopted, the high energy resolution and high time resolution are also required. In this work, the large area $MAPbBr_3$ single crystal has been fabricated with a facile methodology. Due to the quite thick active material and large carrier mobility, the x-ray photons and gamma-ray photons can be absorbed with high efficiency. The photo generated electrons and holes can also be collected effectively with the large electric field. To decrease the dark current in the detection, a novel photo-diode structure is proposed here. In crystallization process of $MAPbI_3$ single crystal, the p-n junction can be formed with doping of selenium atoms into $MAPbI_3$ single crystal.

With various temperature method, the 30mm×30mm×7mm $MAPbBr_3$ single perovskite crystal is fabricated. As the experimental results shown, almost all of the 100 keV x-ray photons are absorbed when the $MAPbBr_3$ SPC is 7mm thick. The detection sensitivity is as high as 305 μC $Gy_{air}^{-1}cm^{-2}$when the anode voltage of x-ray tube is 30 kV .

To reduce the dark current in the detection, two type of photo diode structures have been proposed here. Firstly, a photo diode with structure of Au/TPD/$MAPbBr_3$ PSC/C_{60}/PCBM/Ag has been fabricated with spin coating and sputtering methods. Although the dark current density can be reduced to 20 nA/cm^2 with -30V bias voltage, the temporal response time is nearly 50 μs due to the defects on the interfaces between PSC and carriers transport layers. Then, by doping selenium (Se) in $MAPbI_3$ perovskite single crystals (DPC) crystallization process, low dark current p-n junctions were fabricated without any organic layers. This photodiodes gives the high detection sensitivity as 21000 mC $Gy_{air}^{-1}cm^{-2}$ and 41 mC $Gy_{air}^{-1}cm^{-2}$ for 60 keV x-ray and 1.33 MeV gamma-ray respectively. In this photodiode, the transition time becomes shorter under higher electric field, and the carrier lifetime also becomes shorter due to the dopant of Se atoms. Finally, the temporal response time is measured as 3 μs by experiments. The FWHM width of energy spectrum is decreased to 3.2%@1330 keV.

2D Materials Focus Topic
Room 201B - Session 2D+MI+NS-MoA

2D Materials Characterization including Microscopy and Spectroscopy

Moderators: Stephan Hofmann, University of Cambridge, UK, Richard Vanfleet, Brigham Young University

1:20pm **2D+MI+NS-MoA1 Observing the Mechanisms of Graphene Growth during Chemical Vapor Deposition: Routes to Controlling Layer Number and Domain Size***, Robert Weatherup,* University of Manchester, UK **INVITED**

Chemical vapor deposition (CVD) on polycrystalline metal foils has emerged as the most economic and versatile means for producing 2D materials over large areas,[1] and directly integrating them with other device materials to achieve new functionality.[2] To tailor these materials to specific applications, a detailed understanding of the underlying growth mechanisms is required such that parameters such as domain size, defect density, and layer number can be precisely controlled. However, the elevated temperatures and reactive gas environments involved in growth make direct observation challenging, whilst ex situ measurements are often ambiguous.

Here we apply environmental scanning electron microscopy (ESEM) and ambient pressure X-ray photoelectron spectroscopy (APXPS) to directly observe graphene growth under realistic CVD conditions on polycrystalline Pt foils.[3] This reveals a variety of processes involved in graphene formation including isothermal growth by direct hydrocarbon dissociation, isothermal dissolution into the catalyst bulk, and precipitation on cooling. The balance of these processes, and thus growth outcome, is shown to depends critically on the distribution of carbon close to the catalyst surface, which is in turn is intimately linked to the processing profile.We thereby develop a growth model for graphene CVD that considers precursor dissociation, mass-transport, attachment to the edge of growing graphene domains.[4] This is shown to generally applicable to several transition metal catalysts,[5] and serves as a general framework for understanding and optimizing the growth of 2D materials on polycrystalline catalysts.

We thus demonstrate that the CVD process can be rationally designed to yield different desired growth outcomes from the same polycrystalline starting catalyst, including uniform SLG with large domain sizes (>100 μm), large isolated BLG domains (>50 μm), and uniform BLG. Our result show that through targeted operando experiments the influence of key process parameters can be established, enabling precise control over 2D material growth including domain sizes and layer number.

1. S. Hofmann et al. *J. Phys. Chem. Lett.* **6,** 2714–2721 (2015).

2. M. Piquemal-Banciet al. *Appl. Phys. Lett.* **108,** 102404 (2016).

3. R. S. Weatherupet al. *Nano Lett.* **16,** 6196–6206 (2016).

4. R. S. Weatherupet al. *ACS Nano* **6,** 9996–10003 (2012).

5. A. Cabrero-Vilatela et al. *Nanoscale* **8,** 2149–2158 (2016).

2:00pm **2D+MI+NS-MoA3 Band Alignment of 2-D Materials by Internal Photoemission***, Q. Zhang, S. Zhang,* Theiss Research & National Institute of Standards and Technology*; B. Sperling, **Nhan Nguyen**,* National Institute of Standards and Technology

Two-dimensional (2-D) materials have brought new possibilities for the future electronic and optoelectronic applications [1], [2]. Electronic band alignment at the interface is one of the important parameters in many device designs. For instance, staggered band alignment is preferred to separate photon generated electron-hole pairs in optoelectronic and photovoltaic devices [3]. For the 2-D materials in the monolayer (ML) limit, it has been a challenge to accurately measure the electron affinity which determines how the bands align at the interface. In fact, most 2-D heterojunctions are designed using calculated or theoretically predicted band alignments [4]. In this work, we present an experimental measurement using internal photoemission spectroscopy (IPE) to determine the band offset of MX_2 semiconductors (M = Mo, W; X = S, Se) in relative to an oxide barrier and suggest possible combination of the MX_2 materials to be used for optoelectronic and photovoltaic applications. This IPE approach is seen as a unique method that can be applied to characterize other 2-D materials.

The IPE test structure is fabricated by exfoliating MX_2 flakes on to the Al_2O_3/p^+Si substrate and depositing Ti/Pt contacts on the flakes with large open areas for light absorption. By using gold film mediated exfoliation method [5], large area (> 75 x 75 μm^2) ML MX_2 flakes are obtained, confirmed by Raman spectrum and photoluminescence mapping. Photocurrents of the MX_2-Al_2O_3-p^+Si structure are measure with the incident photon energy swept from 2.0 eV to 5.5 eV and gate voltage V_{GS} (applied to the Si back gate) stepped from -1.0 V to 1.6 V. The oxide flat band voltage (V_{FB}) is extracted by the voltage where the photocurrent switches sign near and above photoemission thresholds. The band offsets at the MX_2/Al_2O_3 and Al_2O_3/Si interfaces are extracted as the thresholds of the cube root of photoemission quantum yield (Y) being the ratio of the photocurrent over the incident light flux [6]. At gate bias below V_{FB}, the band offset between Al_2O_3 and Si is measured and found to be 3.4 eV for all the 4 devices, which is also a well-established value. More importantly, the band offset at the MX_2/Al_2O_3 interfaces combined with the known optical band gaps of ML MX_2 suggest that MoS_2/WS_2 and $MoSe_2/WSe_2$ can possibly form the staggered heterojunction.

[1] G. Fiori, et al, Nat. Nanotech. **9**, 768 (2014).

[2] F. Xia, et al, Nat. Photonics **8**, 899 (2014).

[3] X. Hong, et al, Nature Nanotech. **9**, 682 (2014)

[4] J. Kang, et al, Appl. Phys. Lett. **102**, 012111 (2013)

[5] S. B. Desai, et al, Adv. Mater. **28**, 4053 (2016).

[6] V. V. Afanasev and A. Stesmans, J. Appl. Phys. **102**, 081301 (2007).

2:20pm **2D+MI+NS-MoA4 Visible to mid-IR Nanoscale Characterization of 2D Materials via Photo-induced Force Microscopy***, Padraic O'Reilly, D. Nowak, S. Park,* Molecular Vista

While several 2D materials have been studied with scattering scanning near-field optical microscopes (s-SNOM) with nanoscale spatial resolution, most have focused on the study of surface phonon polariton (SPP) [1]. In this paper, we introduce a relatively new technique called photo-induced force microscopy (PiFM), which combines atomic force microscope (AFM) and broadband optical spectroscopy to analyze both topography and polarizability of samples with sub-10 nm spatial resolution [2]. With PiFM, the near-field optical information is acquired by measuring the photo-induced force between the AFM tip and the sample rather than by collecting photons with a far-field photo-detector; this near-field excitation and near-field detection configuration provides excellent signal-to-noise without the far-field background signal from the much larger focal spot, making the technique robust and easy-to-use. With mid-IR sources, PiFM can image nanoscale SPP as with s-SNOM. With supercontinuum visible-infrared light source, it can directly probe the exciton resonances with equally impressive spatial resolution. With its capability to image number of layers, quality of samples, and plasmonic fields, PiFM is an ideal nanoscale characterization tool for wide range of 2D materials. Results from graphene, MoS_2, WS_2, and hBN will be presented.

[1] T. Low et al., Nature Materials 16, 182–194 (2017).

[2] R. A. Murdick et al., Jap. J. of Appl. Phy., 56, 08LA04 (2017).

2:40pm **2D+MI+NS-MoA5 Polymorphic Structures and Diversified Properties of Low-dimensional Materials Investigated by In situ Electron Microscopy***, Kazu Suenaga,* National Institute of Advanced Industrial Science and Technology (AIST), Japan **INVITED**

Two-dimensional transition metal dichalcogenides (TMDs), consisting of an atomic plane of a transition metal (M: Ti, Nb, Mo, Re, etc.) sandwiched between two chalcogen atomic planes (X: S, Se, Te). This crystalline structure combined with a wide variety of constituent elements give rise to diverse electronic properties, strongly governed by the number of its *d*-orbital electrons. MoS_2 and WS_2 are the most representative "group 6" TMDs featuring trigonal prismatic (H) phase semiconductor with a direct band gap. The TMDs can exhibit various polymorphs and present different electronic properties as the atomic arrangement changes originating from charge transfer. A metallic octahedral (T) phase has been reportedly stabilized by alkali metal intercalation [1], and another distorted octahedral phase zigzag-shape phase (Z) with clusterization of metal atoms into zigzag chains by using solvent-based exfoliation. Some simulations indicate that the Z phase may undergo the Peierls distortion and be transformed into a diamond-shape (DS) phase where atoms reconstruct in a way that four metal atom appear as a diamond (rhombus) in the plane [2]. We show in this talk the experimental evidences for these polymorphic structures and diversified properties found in a family of 2D TMDs.

These monolayer forms in TMDs are typically the same as a single layer of the bulk material. However, $PdSe_2$ presents a puzzle. Its monolayer form has been theoretically shown to be stable, but there have been no reports that monolayer $PdSe_2$ was fabricated. Here, we demonstrate that the preferred monolayer form of this material amounts to a melding of two

bulk monolayers accompanied by the emission of Se atoms so that the resulting stoichiometry is Pd_2Se_3[3].

[1] Y.-C. Lin, D. O. Dumcenco, Y.-S. Huang and K. Suenaga, *Nature Nanotechnology*, 9 (2014) pp.391-396

[2] Y.-C. Lin, H.-P. Komsa, C.-H. Yeh, T. Bjorkman, Z.-Y. Liang, C.-H. Ho, Y.-S. Huang, P.-W. Chiu, A. V. Krasheninnikov, and K. Suenaga, *ACS Nano* 9 (2015) pp.11249-11257

[3] J. Lin, S. Zuluaga, P. Yu, Z. Liu, S. T. Pantelides, and K. Suenaga *Phys. Rev. Lett.*, 119 (2017) 016101

[4] This research was supported by JSPS KAKENHI (JP16H06333 and JP25107003).

3:40pm **2D+MI+NS-MoA8 Probing Interlayer Interaction in van der Waals Materials by Low-energy Electron Microscopy (LEEM)***, **Johannes Jobst**, D. Geelen,* Leiden University, Netherlands*; R.M. Tromp,* IBM, T.J. Watson Research Center*; S.J. van der Molen,* Huygens-Kamerlingh Onnes Laboratory, Netherlands **INVITED**

Knowledge on the interaction between layers is crucial to tailor the properties of van der Waals (vdW) materials. We investigate these using newly developed techniques based on low-energy electron microscopy (LEEM). With LEEM, we probe the reflection of electrons as a function of incoming energy (0-100 eV). We have recently extended our UHV instrument to also measure low-energy electron transmission (eV-TEM).

We apply LEEM and eV-TEM to few-layer graphene. With each layer, an unoccupied interlayer state is added, which hybridizes with the other states. In LEEM, the resulting eigenstates appear as minima in the reflection spectrum. In transmission, they show up as maxima. From both functions, we determine the hybridization energies of the interlayer states, which extend in 2D.

Next, we study the 2D-dispersion relations of these states. For that, we have developed *angle-resolved reflected-electron spectroscopy* (ARRES) [1]. With ARRES, we investigate few-layer graphene, hBN, as well as their combination. For the latter case we find negligible interaction. [2]

[1] Jobst *et al.*, Nat. Comm. **6**, 8926 (2015)

[2] Jobst *et al.,* Nat. Comm. **7**, 13621 (2016)

4:20pm **2D+MI+NS-MoA10 Fast Full Wafer Analysis for Graphene and 2D-materials by Imaging Ellipsometry***, **Sebastian Funke**,* Accurion GmbH, Germany*; P. Braueniger-Weimer, S. Hofmann,* University of Cambridge, UK*; P.H. Thiesen,* Accurion GmbH, Germany

By combining the resolution of optical microscopy and the sensitivity of thin films, imaging ellipsometry (IE) is a powerful tool to characterize thin materials. It allows to measure monolayers of 2D-materials but also to visualize these monolayers on arbitrary substrates. It overcomes the need of specially tuned SiO_2 thicknesses to visualize e.g. Graphene in an optical microscope.

In the talk we present [1], the characterization of Graphene throughout all stages of the manufacturing process from the growth on Cu-foil up to the transferred sample on Si wafers. Unlike other methods IE directly visualizes graphene on the rough Cu. We apply IE to resolve a large area map of Graphene on Cu. The Graphene is directly characterized on the Cu-foil, no oxidation of the Cu is needed. To overcome the waviness of the foil, an autofocus algorithm is developed and applied.

IE is also able to distinguish a Graphene monolayer and hBN monolayer after the transfer process to a Si/SiO_2 substrate. We show large area map of the transfered sample. The contrast mode of IE is able to distinguish the different regions: (a) substrate only, (b) hBN only, (c) Graphene only and (d) an overlapping region of hBN and Graphene. The complete sample approx. 1cm x 0.8 cm is recorded in less than 6 minutes and shows defects and wrapping of hBN of a size as small as 4 µm.

Lastly, we apply IE to characterise full 4'' wafers of graphene on Si.

[1] Braueniger, Funke et al. submitted

Magnetic Interfaces and Nanostructures Division
Room 201A - Session MI+2D+EM+NS-MoA

IoT Session: Symposium on new Magnetic Materials, Devices and Concepts for the Information Society

Moderator: Hendrik Ohldag, SLAC National Accelerator Laboratory

1:20pm **MI+2D+EM+NS-MoA1 "ZOOMING in on Data Storage and the Superb HDD"***, **Roger Wood**,* Western Digital **INVITED**

Get ready for a wild ride starting with the vast distances of outer space and ending with the tiny

distances that separate atoms. For a very different perspective on data storage, each slide in the

presentation looks at things on a scale that is a factor of ten smaller than the previous slide. The

common thread is the technology of information storage. Information storage is what defines human

history and it is the machine-readable data storage developed in the last half-century that provides the

foundation of the modern information age. More than anything, data storage implies magnetic

recording and the hard disk drive. The humble Hard Disk Drive contains such exquisite technologies

and operates at such astounding precision that it almost defies belief. Yet, our industry churns out

these devices by the hundreds of millions and sells them for a few tens of dollars each. Please enjoy

this light-hearted logarithmic romp through storage technology from interstellar space to interatomic

spacings.

(The presentation is based on a talk given at the annual ASME ISPS banquet in Santa Clara, California, in June 2016, while the author was with Western Digital Corporation.)

2:00pm **MI+2D+EM+NS-MoA3 Physics and Applications of Spin-transfer Torques***, **Andrew Kent**,* New York University **INVITED**

The magnetization of a magnetic material can be reversed by using electric currents that transport spin angular momentum [1]. This was predicted in magnetic tunnel junctions—two metallic ferromagnetic layers separated by a thin insulating barrier—by John Slonczewski in 1989 and demonstrated experimentally about a decade later. This discovery has had an enormous impact on magnetism research and technology [2], as prior to this the primary means to reorient the magnetization of a magnet was by applying magnetic fields (dating to 1819 and Oersted!). In this talk I will highlight some of the physics and applications enabled by the discovery of spin-transfer torques. This includes recent experiments that create localized spin-wave excitations (magnons droplets) in thin films with uniaxial magnetic anisotropy [3]. Spin-transfer torques also permit study of magnetic analogues of superconductivity, superfluidity and the Josephson effect that promise to increase our understanding of collective quantum effects. They may even enable braiding Majorana fermions [4]. Finally, I will discuss spin-torque switching of perpendicularly magnetized magnetic tunnel junctions [5], the basic device used in spin-transfer torque magnetic random access memories.

[1] A. Brataas, A. D. Kent and H. Ohno, "Current-Induced Torques in Magnetic Materials," Nature Materials **11**, 372 (2012)

[2] A. D. Kent and D. C. Worledge, "A new spin on magnetic memories," Nature Nanotechnology **10**, 187 (2015)

[3] D. Backes, F. Macia, S. Bonetti, R. Kukreja, H. Ohldag and A. D. Kent, "Direct Observation of a Localized Magnetic Soliton in a Spin-Transfer Nanocontact," PRL **115**, 127205 (2015)

[4] Alex Matos-Abiaguea, Javad Shabani, Andrew D. Kent, Geoffrey L. Fatina, Benedikt Scharfa, Igor Žutić, "Tunable magnetic textures: From Majorana bound states to braiding," Solid State Communications **262**, 1 (2017)

[5] C. Hahn, G. Wolf, B. Kardasz, S. Watts, M. Pinarbasi, A. D. Kent, "Time-resolved studies of the spin-transfer reversal mechanism in perpendicularly magnetized magnetic tunnel junctions," Physical Review B **94**, 214432 (2016)

*Work done in collaboration with Dirk Backes, Gabriel Chaves, Daniel Gopman, Christian Hahn, Jinting Hang, Yuming Hung, Ferran Macia, Daniele Pinna, Laura Rehm, Debangsu Roy, Javad Shabani and Volker Sluka at NYU; Georg Wolf, Bartek Kardasz, Steve Watts and Mustafa Pinarbasi at Spin Transfer Technologies Inc.;and Hendrik Ohldag at SSRL

2:40pm **MI+2D+EM+NS-MoA5 Hybrid Magnetic Heterostructures*, Ivan K. Schuller,*** *A. Basaran,* University of California, San Diego*; J. de la Venta,* Colorado State University*; J.G. Ramirez,* Universidad de los Andes, Colombia*; T. Saerbeck,* Institute Laue-Langevin, France*; I. Valmianski,* University of California, San Diego*; X. Batlle,* University of Barcelona, Spain **INVITED**

Hybrid materials allow the engineering of new material properties by creative uses of proximity effects. When two dissimilar materials are in close physical proximity the properties of each one may be radically modified or occasionally a completely new material emerges. In the area of magnetism, controlling the magnetic properties of ferromagnetic thin films without magnetic fields is an on- going challenge with multiple technological implications for low- energy consumption memory and logic devices. Interesting possibilities include ferromagnets in proximity to dissimilar materials such as antiferromagnets or oxides that undergo metal-insulator transitions. The proximity of ferromagnets to antiferromagnets has given rise to the extensively studied Exchange Bias[1].

In a series of recent studies, we have investigated the magnetic properties of different hybrids of ferromagnets (Ni, Co and Fe) and oxides, which undergo metal-insulator and structural phase transitions. Both the static as well as dynamical properties of the ferromagnets are drastically affected. Static properties such as the coercivity, anisotropy and magnetization [2-3] and dynamical properties such as the microwave response are clearly modified by the proximity effect and give raise to interesting perhaps useful properties.

Work supported by US-AFOSR and US-DOE

Selected References:

[1] *Exchange Bias,*Josep Nogues and Ivan K. Schuller, J. Magn. Magn. Mater. 192, 203 (1999).

[2] *Control of Magnetism Across Metal to Insulator Transitions*, J. de la Venta, Siming Wang, J. G. Ramirez, and Ivan K. Schuller, App. Phys. Lett. 102, 122404 (2013).

[3] *Coercivity Enhancement in V_2O_3/Ni Bilayers Driven by Nanoscale Phase Coexistence*, J. de la Venta, Siming Wang, T. Saerbeck, J. G. Ramirez, I. Valmianski, and Ivan K. Schuller, Appl. Phys. Lett. 104, 062410 (2014).

[4] *Collective Mode Splitting in Hybrid Heterostructures*, Juan Gabriel Ramírez, J. de la Venta, Siming Wang, Thomas Saerbeck, Ali C. Basaran, X. Batlle, and Ivan K. Schuller, Phys. Rev. B, **93**, 214113 (2016).

3:40pm **MI+2D+EM+NS-MoA8 Organismic Materials and Intelligence*, Shriram Ramanathan,*** Purdue University **INVITED**

Intelligence in the natural world is panspermic to life, ranging from basic survival skills in non-neural organisms to co-operative foraging and complex mating strategies in higher level animals. We ask the question whether such remarkable features can be implemented in the physical world utilizing adaptive matter. We have identified strongly correlated semiconductors, one class of quantum materials as particularly suited for this effort, owing to their remarkable electronic plasticity. One may refer to these systems as organismic materials that display certain well-defined characteristics of living beings. In this presentation, we will present examples from the animal kingdom focusing on intelligence and episodic memory. Then we will discuss recent collaborative studies on correlated oxides demonstrating ancestral intelligence. We will conclude with examples of neural networks that can be designed with quantum materials that can replicate fundamental animal learning traits. The role of defects, strain and orbital occupancy control in design of electronic plasticity will be highlighted.

Nanometer-scale Science and Technology Division
Room 102B - Session NS+2D+AS+PC-MoA

SPM - New Imaging and Spectroscopy Methodologies

Moderators: Aubrey Hanbicki, Naval Research Laboratory, Sidney Cohen, Weizmann Institute of Science, Israel

1:20pm **NS+2D+AS+PC-MoA1 A Connection Between Stability of STM Control System and Local Barrier Height: Implications on Imaging and Lithography*, S.O. Reza Moheimani,*** University of Texas at Dallas **INVITED**

Poor performance of the Scanning Tunneling Microscope (STM) control system may result in tip-sample crash, a prevalent failure in STMs. Since its invention, about thirty-five years ago, few attempts have been made to improve the STM control system. Consequently, nearly all STMs are today operated with experimentally selected fixed-gain PI controllers. Selection of controller gains is often done without much attention to the electromechanical dynamics of the scanning tunneling microscope. Performance of such poorly-tuned controllers is limited and a key contributor to the tip-sample crash.

We perform closed loop system identification on a scanning tunneling microscope and show that the system DC gain is proportional to the square root of Local Barrier Height (LBH), a quantum mechanical property of the sample and/or tip that affects the tunneling current. We demonstrate that during a scan the LBH may undergo significant variations and thus it may adversely affect the closed-loop stability if the controller parameters are fixed. Feedback instabilities increase the risk of tip-sample crash in STMs.

In order to improve the closed loop performance, we estimate the LBH, on the fly, and use this information to adaptively tune the PI controller parameters. Experimental results obtained with the self-tuning PI controller confirm the improved STM performance compared to the conventional fixed gain PI controller. Further experiments confirm effectiveness of the proposed method in extending the tip lifetime by lowering the chance of the tip/sample crash.

2:00pm **NS+2D+AS+PC-MoA3 Distinctive Microstructures in a Complex Polymer Evolve with Time and Composition*, x. Yu,*** Worcester Polytechnic Institute*; S. Granados-Focil,* Clark University*; M. Tao, **Nancy Burnham**,* Worcester Polytechnic Institute

The diverse microstructures observed by atomic force microscopy (AFM) in asphalt binder – a complex polymer – suggest complicated intermolecular associations. These microstructures contribute to binders' bulk mechanical properties; therefore, it is essential to understand chemical-microstructural-mechanical relationships for optimal design of binder-related applications, which range from roads to roofs. The US market for asphalt binders in 2019 is predicted to reach 148 million barrels. [1]

Binders annealed at room temperature for over two months showed time-dependent microstructures, which correlate well with room-temperature steric hardening behavior as verified by other researchers using modulated differential scanning calorimetry. Microstructures of the binder films stabilized after different annealing durations, depending on the dimensions of the molecular structures and the complexity of the molecular interactions among the multiple phases in each bitumen. Distinctive microstructures were observed for remixed binders with increasing asphaltene concentrations. Consistency between our observations [2] and other literature suggests that microstructures observed by AFM are probably not just a surface phenomenon.

Furthermore, the complex nature of binder and the various influencing factors often lead to practical challenges in investigation of its microstructures and their chemical origins. Some of the main concerns related to AFM characterization of binders' microstructures, namely the dependence of the microstructures on such factors as sample preparation methods, annealing conditions and durations, and chemical composition, were also addressed in this study.

The above findings provide practical knowledge and deeper insights into the establishment of the complicated chemical-mechanical relationships for asphalt binders that pave the way toward tuned binder performance.

[1] https://www.reportlinker.com/p0158665/US-Asphalt-Industry.html

[2] "Time- and composition-dependent evolution of distinctive microstructures in bitumen." X. Yu, S. Granados-Focil, M. Tao, and N.A. Burnham, Energy Fuels 32, 67-80 (2018).

2:20pm **NS+2D+AS+PC-MoA4 Offering new Characterization Capabilities at the XTIP beamline by Combining Scanning Tunneling Microscopy with Synchrotron Radiation**, ***Volker Rose***, *H. Chang, M. Fisher, S.W. Hla, N. Shirato,* Argonne National Laboratory

The race is on for chemical x-ray imaging with nanoscale resolution. Specifically, there are currently substantial efforts underway at synchrotron facilities worldwide that aim to combine x-rays with scanning probe microscopy. Recently, substantial progress was made on Argonne's Synchrotron X-ray Scanning Tunneling Microscopy (SX-STM) project. SX-STM enables an entirely new view into the nanoworld by combining the best of two worlds: the exceptional chemical, magnetic, and structural sensitivity of synchrotron x-rays combined with the high spatial resolution of scanning probe microscopy accompanied by its ability to engineer and manipulate surfaces down to the level of single atoms.

To fully exploit the special capabilities of a unique new cryogenic x-ray microscope, XTIP, a dedicated beamline for SX-STM will become available at the Advanced Photon Source in early 2019. To meet the scientific objective of the nanoscience and nanomagnetism communities most effectively, we are going to build a soft x-ray beamline with full polarization control operating over the 500-1600 eV energy range. The dedicated XTIP beamline will provide researchers access to a one-of-a-kind instrument. Among the potential breakthroughs are "designer" materials created from controlled assembly of atoms and molecules, and the emergence of entirely new phenomena in chemistry and physics.

2:40pm **NS+2D+AS+PC-MoA5 Scanning Probe Microscopy Based Spectroscopy Measurement for Nanoscale Chemical Identification**, ***Chanmin Su***, Bruker-Nano, Inc. **INVITED**

Scanning probe microscopy has been instrumental for physical property characterizations at the nanometer scale, primarily for mechanical, electromagnetic and thermal properties. Recent progresses were focused on chemical identification based on mid-IR spectroscopy, pushing FTIR mapping to a resolution at or beyond 10 nm. This presentation will review technology advances in both scanning near field optical microscopy and photothermal based IR spectroscopy. Each of the techniques is discussed and benchmarked by detection limit, spatial resolution and signal to noise ratio, which ultimately determines the chemical mapping efficiencies. We will highlight techniques that address correlative imaging where physical and chemical properties at the same nanoscale location being acquired either concurrently or sequentially. As an example, PeakForce tapping based chemical and physical measurements will be explained in detail with the applications ranging from 2D materials to polymer complexes. The presentation will also highlight major challenges for scanning probe based measurements to be broadly adopted as the premier tool for nanoscale chemical fingerprint mapping.

3:40pm **NS+2D+AS+PC-MoA8 Quantifying Tip-Sample Interactions in Vacuum Using Cantilever-based Sensors: An Analysis**, *O.E. Dagdeviren, C. Zhou, E.I. Altman,* ***Udo D. Schwarz***, Yale University

To achieve as much quantitative information on a surface as possible, the local measurement of tip-sample interaction potentials has recently gained much popularity in particular under well-defined ultrahigh vacuum conditions, where such measurements can be carried out with great accuracy both in terms of spatial as well as force resolution. To this end, either the oscillation frequency or the oscillation amplitude and phase of the vibrating force-sensing cantilever are recorded as a function of tip-sample distance and subsequently converted into quantitative values for the force or interaction potential. Here, we theoretically and experimentally show that the force law obtained from such data acquired under vacuum conditions using the most commonly applied methods may deviate more than previously assumed from the actual interaction when the oscillation amplitude of the probe is of the order of the decay length of the force near the surface, which may result in a non-negligible error if correct absolute values are of importance [1]. Caused by approximations made in the development of the mathematical reconstruction procedures, the related inaccuracies can be effectively suppressed by using oscillation amplitudes sufficiently larger than the decay length. To facilitate efficient data acquisition, we propose a novel technique that includes modulating the drive amplitude at a constant height from the surface while monitoring the oscillation amplitude and phase.Ultimately, such amplitude sweep-based force spectroscopy enables shorter data acquisition times and increased accuracy for quantitative chemical characterization compared to standard approaches that vary the tip-sample distance. An additional advantage is that since no feedback loop is active while executing the amplitude sweep, the force can be consistently recovered deep into the repulsive regime.

[1] O. E. Dagdeviren et al., Physical Review Applied **9**, 044040 (2018).

4:00pm **NS+2D+AS+PC-MoA9 AFM + Nanoscale Vis-IR Spectroscopy via Photo-induced Force Microscopy**, ***Derek Nowak***, *T. Albrecht, S. Park,* Molecular Vista

Photo-induced Force Microscopy (PiFM) [1] combines optical spectroscopy and atomic force microscopy (AFM) via illumination of the tip-sample junction with tunable laser light and mechanical detection of forces acting on the tip in response to interaction of light with the sample. With infrared (IR) source, PiFM can map the IR absorption of the sample as a function of IR wavelength and position and achieve nm-scale resolution in displaying the locations of heterogeneous materials on the surface of a sample. Even for samples without active IR absorption band, PiFM can be used to acquire nanoscale mapping based on the dielectric constant of the sample surface; dielectric constant mapping also allows high resolution sub-surface mapping. With tunable visible and near infrared (VisNIR) laser source, PiFM can map exciton resonances with similar spatial resolution even on monolayer samples. Examples from various classes of samples including organic, inorganic, and 2D materials will be presented. We will also present PiFM spectroscopy data that show excellent correlation with bulk FTIR spectra despite the fact that PiFM acquires local chemical information from regions in the range of 10 nm in extent.

[1] D. Nowak et al., Sci. Adv. **2**, e150157 (2016).

2D Materials Focus Topic
Room 201B - Session 2D+EM+MI+NS-TuM

Properties of 2D Materials including Electronic, Magnetic, Mechanical, Optical, and Thermal Properties

Moderator: Johannes Jobst, Leiden University

8:00am **2D+EM+MI+NS-TuM1 Effect of Lattice Stacking Orientation and Local Thickness Variation on the Mechanical Behavior of Few Layer Graphene Oxide**, ***Teng Cui***, *S. Mukherjee, C.H. Cao, P.M. Sudeep, J. Tam,* University of Toronto, Canada*; P.M. Ajayan,* Rice University*; C.V. Singh, Y. Sun, T. Filleter,* University of Toronto, Canada

Investigation of few layer 2D materials is fundamentally important to bridge the gap between monolayer and bulk properties, and practically meaningful for applications as reinforcement nanofillers and layered electronic devices. Few layer introduces differences from intrinsic properties of monolayers due to the complexity of structural heterogeneities, such as lattice stacking orientation and local thickness variation. In this work [1], few layer graphene oxide (GO) with different structural heterogeneities were studied using atomic force microscopy-based deflection measurements and transmission electron microscopy (TEM). Direct TEM evidence of fracture surfaces and molecular dynamics (MD) simulations revealed decoupled and dissimilar layer crack patterns (i.e., different cracking pathway of top and bottom layers) for misaligned bilayer GO. In contrast, aligned GO bilayers generally fractured with a larger portion of common cracks shared by both layers, indicating stronger interlayer interaction than its misaligned counterpart. MD results also revealed insignificant effect of lattice alignment on the strength and toughness of GO bilayers, which is ~23.5 GPa and ~1.71×10^{-18} J/nm^3, respectively, for both aligned and misaligned cases. Scaling up to ~5 layers and above revealed more significant local thickness heterogeneity and consequently a ~60% reduction of the normalized fracture force and toughness with respect to the average number of layers. MD simulations on partially intercalated few layer GO revealed anisotropic and heterogeneous stress distributions, as well as stress concentration near the inner edges, which may account for the significant reduction of strength and toughness.

[1] T. Cui, S. Mukherjee, C. Cao, P. M. Sudeep, J. Tam, P. M. Ajayan, C. V. Singh, Y. Sun, and T. Filleter, "*Effect of Lattice Stacking Orientation and Local Thickness Variation on the Mechanical Behavior of Few Layer Graphene Oxide*", **Carbon**, accepted.

8:20am **2D+EM+MI+NS-TuM2 Out-of-Plane Mechanical Properties of 2D Hybrid Organic-Inorganic Perovskites by Nanoindentation**, ***Qing Tu***, *I. Spanopoulos, S. Hao, C. Wolverton, M. Kanatzidis, G. Shekhawat, V. Dravid,* Northwestern University

2D layered hybrid organic-inorganic perovskites (HOIPs) have demonstrated improved stability and promising photovoltaic performance. The mechanical properties of such functional materials are both fundamentally and practically important to achieve both high performance and mechanically stable (flexible) devices. Here we report the static, out-of-plane mechanical properties of a series of 2D layered lead iodide HOIPs with a general formula of $(R\text{-}NH_3)_2(CH_3NH_3)_{n-1}Pb_nI_{3n+1}$, and investigate the role of structural sub-units (*e.g.*, the length of theorganic spacer molecules -R and the number of inorganic layer -n) on the mechanical properties by nanoindentation. We find that the 2D HOIPs are softer than their 3D counterparts due to the replacement of the strong inorganic layer and ionic bonds by the soft organic layers and the weak Van der Waals interactions. As n increases from 1 to 5, the relative amount of these weak factors in the crystals are decreasing and both the out-of-plane Young's modulus E and hardness H increase, approaching to the reported values of corresponding 3D crystals. DFT simulations showed a similar trend to the experimental results. Furthermore, we show that increasing the alkyl chain spacer molecule -R from $-C_4H_9$ to $-C_{12}H_{25}$, E first decreases and eventually plateaus while no clear trend in H is observed. Our results reveal that the competition between the stiff inorganic layers, the soft organic layer and the weak Van der Waals interfaces determines the mechanical properties of 2D HOIPs. Finally, we compare these findings with those in other 2D layered materials such as h-BN, MoS_2 and MXene, and shed light on routes to further tune the out-of-plane mechanical properties of 2D layered HOIPs.

8:40am **2D+EM+MI+NS-TuM3 Mechanical Properties of Many-layer CVD Graphene**, ***Kyle Larsen***, *S. Lehnardt, J.T. Rowley, B. Anderson, R.R. Vanfleet, R.C. Davis,* Brigham Young University

Graphene, a monoatomic layer of carbon atoms, has a reported Young's modulus of 1 TPa and a tensile strength of 130 GPa. These values make it both the strongest and one of the stiffest materials ever reported. The mechanical properties of multilayer graphene grown by chemical vapor deposition have been reported for films of up to 10 layers (3.35 nm). Films thicker than about 10 layers (sometimes considered graphite rather than multilayer graphene) are of interest as membranes and in MEMS applications. We have characterized CVD grown many-layer graphene films with thicknesses of about 50 nm by Raman spectroscopy, burst testing, and atomic force microscopy. The atomic force microscope was used to map the local compliance over suspended regions containing cantilevers cut out of the many-layer graphene with a focused ion beam. Analytical and finite element modeling were used in the analysis of the deflection of the many-layer graphene cantilevers to extract Young's modulus. The many-layer graphene is high quality (little or no D peak in the Raman spectrum) and has a Young's modulus in the range reported for graphene (0.5 TPa to 1 TPa).

9:20am **2D+EM+MI+NS-TuM5 Discovering and Visualizing Ferromagnetism in Intrinsic Two Dimensional Materials**, ***Jing Xia***, University of California Irvine **INVITED**

In this talk, I will discuss our recent results on discovering and visualizing in 2D magnetism using a unique scanning Sagnac MOKE microscope, which is based on a Sagnac interferometer technique and has achieved unprecedented nano-radian level Kerr and Faraday sensitivity even at DC. In exfoliated Cr2Ge2Te6 (CGT) atomic layers, we report the discovery of intrinsic ferromagnetism in 2D van der Walls crystals, defying the well-known Mermin-Wagner theorem. Unlike 3D magnetism, the ferromagnetic order in this 2D system is stabilized by magnetic anisotropy from the CGT structure, which is not present in graphene. As a result, changing the magnetic anisotropy with a small external magnetic field was found to strongly enhance the Curie temperature, which is a feature unique to 2D magnetism.

11:00am **2D+EM+MI+NS-TuM10 Onset of Buckling Folding and Slipping Instabilities in 2D Materials under Compressive Strain**, ***Jaehyung Yu***, *E. Ertekin, A.M. van der Zande,* University of Illinois at Urbana-Champaign

Atomic membranes of monolayer 2D materials represent the ultimate limit in size of nanoelectromechanical systems. These materials have high mechanical strength, yet low bending modulus leading to high pliability. Adding in the diverse active electronic properties of different 2D materials, atomic membranes will allow new next generation technologies like highly strainable crumpled or folded electronics, or 3D origami devices based on 2D materials. In order to realize these new technologies it is important to understand how the rules of continuum membrane mechanics break down on the atomic scale and how these deformations will affect the electronic properties, including the role of compressive stress, bending, adhesion and interlayer shear.

Here, we present a combined experimental and theoretical study of the onset of instabilities such as buckling, folding and slip on the properties of 2D materials and heterostructures under compression. We generate periodic fold structures of the graphene, MoS2, and their heterostructures by introducing the compressive stresses with the pre-strained stretchable substrate. We analyzed then measured the membrane morphology using atomic force microscopy (AFM) under increasing levels of uniaxial compression up to 30%. We observed that the strain-relaxation mechanism of atomic membranes could be varied from generating and growing standing folds to collapsing to generate trifolds based on the mechanical properties including 2D modulus, bending stiffness, adhesion and interlayer shear energies. The onset of these instabilities depends on the 2D material or heterostructure making up the membranes. In graphene folds grow then collapse at compressive strain of ~5%. In monolayer MoS2 standing folds grow to a fixed height of ~20 nm but do not collapse. Instead, new folds are generated in between the existing folds.

We use density functional theory (DFT) to model the morphology of the same structures under compressive slack. We find that, in multi-layer 2D materials, the onset of slip between the layers is crucial parameters to decide the bending stiffness of the material. We found that the superlubricity between the layers allows the linear scaling of bending stiffness with the number of layers, which violates the conventional cubic scaling of bending stiffness in continuum mechanics.

We unite the atomic scale simulation with the experiment through a continuum model to compare the period, shape, and transition strains extract the variations in adhesion and bending energy of different 2D materials and heterostructures to find the deformation of 2D materials under the compressive strain.

11:20am **2D+EM+MI+NS-TuM11 Title: Spatially-Resolved Contact-Free Electrical Characterization of Transition Metal Dichalcogenide Films Grown by Chemical Vapor Deposition.***, **Miguel Isarraraz**, L. Bartels,* University of California, Riverside

Surface Acoustical Waves (SAWs) and Transition Metal Dichalcogenides (TMDs), separately, are topics of current research due to their present and future use in telecommunications and beyond-CMOS technology. The interaction between a SAW and a 2D electron gas has been previously studied by measuring the absorption of the SAW by GaAs and, more recently, graphene[i,ii,ii]. Here, the interaction between a SAW and a TMD is studied using MoS_2 directly grown by chemical vapor deposition on 128°YX-cut $LiNbO_3$. By focusing a 532 nm laser on the sample, the generation of electron-hole pairs is found to enhance the attenuation of the SAW as expected, and this technique can be used to spatially resolve variations inside triangular MoS_2 islands. Furthermore, the time dependence of the SAW attenuation with laser exposure is used to distinguish between heating and electronic effects. The induced acoustoelectric current, laser power, and SAW excitation power dependence are discussed. This technique provides a means of electrically characterizing atomically thin semiconducting film that avoids the limitations of metallic contacts.

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11:40am **2D+EM+MI+NS-TuM12 Electronic, Thermal, and Unconventional Applications of 2D Materials***, **Eric Pop**, E. Yalon, C. McClellan, K. Smithe, C. English, M. Mleczko, M. Muñoz Rojo, N. Wang, S. Suryavanshi, I. Datye, C. Bailey, A. Gabourie, M. Chen, V. Chen, K. Schauble, R. Grady,* Stanford University **INVITED**

This talk will present recent highlights from our research on two-dimensional (2D) materials and devices including graphene, boron nitride (h-BN), and transition metal dichalcogenides (TMDs). The results span from fundamental measurements and simulations, to devices, to system-oriented applications which take advantage of unusual 2D material properties. On the fundamental side, we have measured record velocity saturation in graphene [1,2], as well as the thermal properties of graphene nanoribbons [3]. These are important for electronic applications, which can exhibit substantial self-heating during operation [4]. Taking advantage of low *cross-plane* thermal conductance, we found unexpected applications of graphene as ultra-thin electrode to reduce power consumption in phase-change memory [5]. We have also demonstrated wafer-scale graphene systems for analog dot product computation [6].

We have grown monolayer 2D semiconductors by chemical vapor deposition over cm^2 scales, including MoS_2 with low device variability [7], WSe_2, $MoSe_2$ – and multilayer TMDs $MoTe_2$ and WTe_2 [8]. Importantly, $ZrSe_2$ and $HfSe_2$ have native high-K dielectrics ZrO_2 and HfO_2, which are of key technological relevance [9]. Improving the electrical contact resistance [10], we demonstrated 10 nm transistors using *monolayer* MoS_2, with the highest current reported to date (>400 µA/µm), approaching ballistic limits [11]. Using Raman thermometry, we uncovered low thermal boundary conductance (~15 $MW/m^2/K$) between MoS_2 and SiO_2, which could limit heat dissipation in 2D electronics [12]. We are presently exploring unconventional applications including thermal transistors [13], which could enable nanoscale control of heat in "thermal circuits" analogous with electrical circuits. Overall, these studies reveal fundamental limits and new applications that could be achieved with 2D materials, taking advantage their unique properties.

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2D Materials Focus Topic
Room 201B - Session 2D+EM+MI+MN+NS-TuA

2D Device Physics and Applications

Moderator: Roland Kawakami, The Ohio State University

2:20pm **2D+EM+MI+MN+NS-TuA1 Spin Relaxation and Proximity Effect in WS_2/Graphene/Fluorographene Non-local Spin Valves**, ***Adam Friedman,*** Laboratory for Physical Sciences*; K.M. McCreary, J.T. Robinson, O.M.J. van 't Erve, B.T. Jonker,* US Naval Research Laboratory

The mechanisms leading to spin relaxation in graphene and its heterostructures continue to be debated. Control of the spin relaxation in graphene-based structures is necessary to achieve the envisioned utility of graphene in future spintronic devices beyond Moore's law. Proximity induced spin relaxation caused by contact to a high spin-orbit material, such as WS_2, offers a promising avenue to manipulate the spin lifetime [1]. We demonstrate the operation of WS_2/graphene/fluorographene non-local spin valves and extract the spin lifetimes for a range of carrier concentrations by Hanle effect measurements. Four-terminal charge transport measurements allow us to calculate the momentum relaxation time as a function of carrier concentration and compare it to the spin lifetime. These data show that the D'yakonov-Perel' mechanism is the dominant spin relaxation mechanism for WS_2/graphene/fluorographenedevices, while, for reference graphene/fluorographene devices, linear scaling between the spin and momentum lifetimes points to spin-flip scattering during strong elastic scattering events where the scattering event is strongly coupled to the electron spin. We attribute the change in spin relaxation type in part with the inclusion of WS_2 as a substrate to proximity induced spin-orbit coupling due to the adjacent WS_2 layer, and we compare our data to the literature.

[1] A.L. Friedman, et al. Carbon 131, 18-25 (2018).

2:40pm **2D+EM+MI+MN+NS-TuA2 Two-dimensional Field-effect Light Emitting Transistors**, ***Junyoung Kwon,*** *H. Ryu,* Yonsei University, Republic of Korea*; J.Y. Lee, C.H. Lee,* Korea University, Republic of Korea*; G.H. Lee,* Yonsei University, Republic of Korea

Two dimensional (2D) materials and their heterostructures hold great promises in various applications due to their unique properties and newly discovered physics. Especially, high exciton binding energy and emergence of charged excitons, *i.e.* trions, have shown that 2D semiconductors, such as transition metal dichalcogenides (TMDs), are promising candidates for new concept optoelectronics. Although lots of optoelectronic devices based on the van der Waals heterostructures of 2D materials, such as photodetectors, solar cells, and light emitting devices, have been demonstrated, development of novel optoelectronic devices is still required to fully utilize unique properties of 2D materials and enable multi-functions and versatile applications. Here we demonstrate 2D filed-effect light emitting transistors (2D-FELET) consisting of monolayer WSe_2 (light-emitting channel layer) and graphene contacts (tunable carrier injection electrodes). We encapsulated monolayer WSe_2 with two pieces of hexagonal boron nitride and fabricated graphene contacts to two ends of WSe_2. To selectively inject different types of charge (electrons and holes) at two graphene contacts, two separate top gates on top of WSe_2-graphene overlap regions were fabricated. By independent modulation of two top gates, Schottky barrier heights for electrons and holes can be tuned, which enables the selective charge injections. When two top gates are oppositely biased, electrons can be injected from one end of WSe_2 channel and holes can be injected from the other end. These opposite charges are recombined at the middle of WSe_2 channel, leading to strong light emission. The performance of the 2D-FELETs is tunable by additional electrical field from back gate. Furthermore, the devices produced in this work can be used as polarity-tunable FETs and photodetectors, simultaneously, which are beneficial for further CMOS integration. Our study shows great potential of 2D-FELETs toward future optoelectronic applications, which request ultra-thinness, transparency, flexibility, high efficiency, multi-functions, and high integration.

3:00pm **2D+EM+MI+MN+NS-TuA3 Quantum Devices with 2D Materials**, *H. Overweg, M. Eich, R. Pisoni, T. Ihn, P. Rickhaus,* ETH Zurich, Switzerland*;* ***Klaus Ensslin,*** ETH Zürich, Switzerland **INVITED**

Quantum dots in graphene have been mostly realized by etching. This leads to localized states at the uncontrolled edges dominating the transport properties of these quantum devices. [1] It is well known that in bilayer graphene gaps can be opened by vertical electrical fields. [2] This approach has been used with limited success to define quantum devices [3]. The pinch-off characteristics are typically limited by leakage currents often thought to occur at the physical sample edges [4].

Here we demonstrate that electrostatically tunable barriers can be fabricated on bilayer graphene devices with graphite as a back gate. We measure pinch-off resistances exceeding GOhms and observe quantized conduction plateaus for one-dimensional constrictions. [5] With suitable gate arrangements few carrier hole and electron quantum dots can be electrostatically defined. We measure the controlled occupation of quantum dots with single holes and electrons. Four-fold level bunching is observed in Coulomb blockade spectroscopy which is understood in terms of valley and spin states. Magnetic field dependence allows to investigate orbital and spin/valley degrees of freedom.

We further demonstrate quantum devices build on MoS2.

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2. Oostinga et al., Nat. Materials 7, 151 (2007)

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5. Overweg et al., [https://arxiv.org/abs/1707.09282], [https://arxiv.org/abs/1709.00870]

4:20pm **2D+EM+MI+MN+NS-TuA7 GaN Microdisk Light-emitting Diode Display Fabricated on Graphene**, ***Youngbin Tchoe,*** *K. Chung, K. Lee, M.S. Song, J.B. Park, H. Kim, J.Y. Park, G.-C. Yi,* Seoul National University, Republic of Korea

Microdisplay with high resolution, brightness, and efficiency with long-term stability and reliability are highly required for advanced display technologies. Inorganic semiconductors LEDs best suits this purpose because they can emit very high density of light from a small area and they have very high efficiency and long-term stability. To use inorganic LEDs for display applications, various lift-off and transfer techniques of inorganic thin films grown on single crystal substrates, such as sapphire or Si, were developed. However, achieving display devices using inorganic semiconductor thin films is still very challenging because of the limited size and high manufacturing cost of the single crystal substrates, as well as the complicated processes required for lift-off and assembly. To resolve this problem, growths of inorganic semiconductor nanostructures and thin films on graphene substrates have recently been proposed, since graphene has great scalability and extremely thin layered hexagonal lattice structure as an excellent substrate for GaN growth. Moreover, the inorganic semiconductors prepared on large-area graphene can be transferred easily to or grown on elastic substrates to meet the flexibility demand. Here, we suggest a method of fabricating ultrathin, high-resolution inorganic microdisplay based on individually addressable GaN microdisk LED arrays grown on graphene dots.

Here, we report on the fabrication and EL characteristics of ultrathin and individually addressable GaN microdisk LED arrays grown on graphene dots for microdisplay applications. GaN microdisks were prepared by epitaxial lateral overgrowth on patterned graphene microdots on SiO_2/Si substrates using MOVPE. After preparing the GaN microdisk arrays, *p*-GaN and InGaN/GaN multiple quantum well, and *n*-GaN layers were heteroepitaxially grown on the surface of the GaN microdisks. Ultrathin layers composed of GaN microdisk LED arrays on graphene dot were prepared by coating a polyimide layer and lifting-off the entire layers from the substrate. Then, single-walled carbon nanotubes (SWCNTs)/Ni/Au and SWCNTs/Ti/Au multiple electrode lines were formed on the top and bottom surface of GaN microdisk arrays in an aligned manner and crossing each other. The electrical and optical characteristics of the individually addressable GaN microdisk array on graphene dots were investigated by measuring their *I–V* curves and EL characteristics at various bending conditions. We also confirmed that the ultrathin micro-LED display worked reliably under flexible conditions and continuous operation mode.

4:40pm **2D+EM+MI+MN+NS-TuA8 Room Temperature Magnetron Sputtering and Laser Annealing of Ultrathin MoS_2 for Transistor Device Fabrication on Flexible Polymer Substrates**, ***Benjamin Sirota,*** University of North Texas*; N.R. Glavin,* Air Force Research Laboratory*; C. Arnold, A.A. Voevodin,* University of North Texas

Pulsed magnetron sputtering and subsequent laser annealing provide technologically attractive scalable route for producing two-dimensional (2D) semiconducting grade MoS_2 materials directly on the surface of flexible polymer substrates. In this study the room temperature magnetron sputtering was used to deposit 10 nm thick, amorphous MoS_2 films on

flexible PDMS as well as rigid SiO_2/Si substrates. This was followed by 248 nm pulsed laser annealing to produce polycrystalline 2H-MoS_2 over large areas. Raman and XPS analysis confirmed that pulsed laser annealing with about 1 mJ/cm^2 energy density had induced film crystallization from amorphous to hexagonal, while preserving MoS_2 chemical composition, and avoiding formation of oxide phases or damage to the temperature-sensitive polymer surface. Electrical measurements confirmed an order of magnitude improvement in electrical conductivity of the laser annealed films as compared to amorphous MoS_2. Top-gated field effect transistor (FET) devices with laser annealed sputter grown MoS_2 were directly fabricated on PDMS surfaces. Oxygen substitution of sulfur in sputter deposited MoS_2 and polycrystallinity of the laser annealed 2H-MoS_2 films resulted in low mobility values when compared to mechanically exfoliated and chemical vapor deposition grown single-crystal 2D MoS_2. However, the described approach is intrinsically scalable and provides a direct growth route for the fabrication of 2D transition metal dichalcogenide semiconducting devices on the surface of flexile and stretchable polymers.

5:00pm **2D+EM+MI+MN+NS-TuA9 Black Phosphorus: Fundamental Properties and Emerging Applications***, **Han Wang,*** University of Southern California **INVITED**

In this talk, I will discuss our recent work in developing novel electronic and photonic devices based on the anisotropic properties of black phosphorus (BP) and its isoelectronic materials such as the monochalcogenides of Group IV elements. High mobility, narrow gap BP thin film (0.3 eV in bulk) fill the energy space between zero-gap graphene and large-gap TMDCs, making it a promising material for mid-infrared and long wavelength infrared optoelectronics. Most importantly, its anisotropic nature within the plane of the layers allow for the realization of conceptually new electronic and photonic devices. Here, I will first present our work in understanding the fundamental electronic and optical properties of black phosphorus using a newly developed scanning ultrafast electron microscopy (SUEM) technique and photoluminescence spectroscopy. Our recent the study of bandgap tuning in BP and the demonstration of a polarization sensitive BP mid-IR detector will then be presented. In the second half of my talk, I will discuss our work on developing two dimensional materials based artificial synaptic devices for neuromorphic electronics, including emulating the heterogeneity in synaptic connections using the anisotropic properties of BP and a tunable memristive device as a reconfigurable synapse. I will conclude with remarks on promising future research directions of low-symmetry electronics based on anisotropic 2D materials and how their novel properties is expected to benefit the next-generation electronics and photonics technologies.

5:40pm **2D+EM+MI+MN+NS-TuA11 Patterned Growth of Hybrid Bulk-2D Tungsten Diselenide for Transistor Applications***, **Quinten Yurek**, I. Liao, D. Barroso, A.E. Nguyen, N. Duong, G. Stecklein, L. Bartels,* University of California, Riverside

As device dimensions shrink, surfaces and interfaces between materials make up a larger volume fraction of a device leading to degrading device properties in 3D materials. One solution is to use 2D materials, however these materials introduce additional challenges. For instance, high resistance Schottky barriers and a small number of free charge carriers in comparison to bulk materials. The effective mobility of field effect transistors (FETs) based on two-dimensional (2D) single-layer transition metal dichalcogenide (TMD) films is frequently limited by barriers at the contacts, as opposed to the native properties of the TMD material. Specifically, high resistance Schottky barriers form at the TMD/metal interface because of the film's thinness and resulting small number of carriers. Here we demonstrate a scalable single-step deposition method for nanoscale hybrid 2D/3D TMD structures encoded by lithographic patterning prior to deposition. By confining the metal contact to the bulk regions of WSe_2, the effective mobility is increased to nearly 100 cm^{2}V^{-1}s^{-1} with an on/off ratio >10^5 for bottom-gated devices (through 300nm of oxide), even for comparatively long channels (>5 microns) and absent other contact optimization. Our process involves lithographic patterning of a hafnium (IV) dioxide film onto the SiO_2/Si substrate prior to TMD growth. Bulk-like 3D WSe_2 is observed to grow at the location of the hafnia, while 2D single-layer material is grown in regions of bare SiO_2. Systematic evaluation of transport data allows us to extract Schottky barrier heights and other fundamental properties of our hybrid devices. We demonstrate that this process can be used to create devices with metal/3D TMD contacts, which exhibit a reduced Schottky barrier height, while continuing to use 2D TMD channels, which result in an excellent on-off ratio.

6:00pm **2D+EM+MI+MN+NS-TuA12 Enhanced Ionic Sensitivity in Solution-Gated Graphene-Hexagonal Boron Nitride Heterostructure Field-Effect Transistors***, A.D. Radadia, **Nowzesh Hasan**, B. Hou, A.L. Moore,* Louisiana Tech University

The charge transport in solution-gated graphene devices is affected by the impurities and disorder of the underlying dielectric interface and its interaction with the solution. This paper reports advancement in field-effect ion sensing by fabricating a dielectric isomorph, hexagonal boron nitride between graphene and silicon dioxide of a solution-gated graphene field effect transistor. Ionic sensitivity of Dirac voltage as high as -198 mV/decade for K^+ and -110 mV/decade for Ca^{2+} were recorded. Increased transconductance due to increased charge carrier mobility was accompanied with larger ionic sensitivity of the transconductance due to larger ionic sensitivity of the charge carrier mobility. These findings define a standard to construct future graphene devices for biosensing and bioelectronics applications.

Electronic Materials and Photonics Division
Room 101A - Session EM+2D+AN+MI+MP+NS-TuA

Solar/Energy Harvesting and Quantum Materials and Applications

Moderators: Yohannes Abate, Georgia State University, Nicholas Strandwitz, Lehigh University

2:20pm **EM+2D+AN+MI+MP+NS-TuA1 Plasmonic Metasurface Electrodes for Excitonic Solar Cells.***, **Deirdre O'Carroll,*** Rutgers, the State University of New Jersey **INVITED**

Excitonic organic solar cell technologies, while not currently competitive with inorganic-semiconductor analogues, can exhibit very small device embodied energies (due to comparatively low temperature and low energy-use fabrication processes), which is of interest for minimizing overall device cost and energy-payback time. To improve energy conversion efficiency in thin-film excitonic organic solar cells, light management using nanophotonic structures is necessary. Here, our recent work on improving light trapping in deeply-subwavelength excitonic organic semiconductor films using plasmonic metasurfaces will be presented. Numerous exciton-metasurface interaction phenomena, such as absorption-induced scattering, exciton-plasmon coupling and morphology-dependent surface plasmon light-trapping are observed to give rise to improved light trapping at different regions of the solar spectrum. Additionally, an approach to achieve the theoretical limits to the efficiency of excitonic organic photovoltaics (~22%) will be proposed that involves control of radiative recombination rate, and optimization of both photoluminescence quantum efficiency and photon recycling in organic semiconductor thin-films.

3:00pm **EM+2D+AN+MI+MP+NS-TuA3 Photoemission Electron Microscopy as a New Tool to Study the Electronic Properties of an Inhomogeneous Semiconductor for Photovoltaics***, M. Berg,* Sandia National Laboratories*; J. Kephart, A. Munshi, W.S. Sampath,* Colorado State University*; **Taisuke Ohta**, C. Chan,* Sandia National Laboratories

The energy positions of the valence and conduction electronic states with respect to the vacuum level are essential parameters to evaluate how the band gaps of semiconductors or Fermi-levels of metals line up with respect to each other. Such electronic structures of materials can be determined using photoemission spectroscopy (PES). PES measurements, however, remain challenging for inhomogeneous materials with nano- to micrometer lateral dimensions due to its mesoscopic probing area, typically no less than several microns. Photoemission electron microscopy (PEEM) is a cathode lens electron microscopy technique that combines photoemission imaging with spectroscopic modes of operation to provide PES spectra from areas less than one micron in size. Here, we present PEEM studies of the electronic structure of polycrystalline cadmium telluride (CdTe) thin films, a test case to examine the applicability of this new microscopic approach to photovoltaic materials. Post-deposition $CdCl_2$ treatment of CdTe is known to increase photovoltaic efficiency. However, the precise chemical, structural, and electronic changes that underpin this improvement are still debated. In this study, PEEM was used to spatially map the vacuum level and ionization energy of CdTe films, enabling the identification of electronic structure variations between grains and grain boundaries. *In vacuo* preparation and inert environment transfer of oxide-free CdTe surfaces isolated the separate effects of $CdCl_2$ treatment and ambient oxygen exposure. Qualitatively, grain boundaries displayed lower

work function and downward band bending relative to grain interiors, but only after air exposure of $CdCl_2$-treated CdTe. This study highlights the importance of probing the spatially varying electronic structure, elucidating the concurrent impacts of processing steps ($CdCl_2$ treatment and oxygen exposure) to develop a comprehensive picture of local electronic structure in an inhomogeneous semiconductor.

The PEEM work was performed at the Center for Integrated Nanotechnologies, an Office of Science User Facility (DE-AC04-94AL85000). M. B. & C. C. were supported by a U.S. DOE-EERE SunShot BRIDGE award (DE-FOA-0000654 CPS25859). T. O. was supported by the CINT user program and Sandia LDRD. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the US DOE or the US Government.

3:20pm **EM+2D+AN+MI+MP+NS-TuA4 Modification of Bandgap for Lead-Free Double Perovskite $Cs_2AgInCl_6$ with Bi Doping**, ***Hassan Siddique***, *H. Da, X.Q. Wang, R.C. Dai, Z.P. Wang, Z.J. Ding, Z.M. Zhang,* University of Science and Technology of China

Lead halide perovskites have the excellent luminescent properties but exist some vital disadvantages such as instability and Pb toxicity. Lead-free double perovskites draw attention due to a possible candidate for environment-friendly materials. Direct bandgap lead-free halide of $Cs_2AgInCl_6$ is one of them. [1] In this work Bi doping $Cs_2AgInCl_6$ (CAIC) was successfully prepared. Bi dopant above 15% CAIC can restrict the parity forbidden transition responding to sub absorption peak around 600 nm.[2] On the other hand, the intensity of photoluminescence enhances with the increasing Bi dopant and touches the maximum around 30% doping, then gradually loses its intensity with further doping due to the mechanism of the concentration quenching at room temperature. Bi doping in CAIC can also modify the band gap. The absorption spectra indicate that the band gap reduces from 3.10eV without Bi doping to 2.68eV for $Cs_2AgIn_{0.30}Bi_{0.70}Cl_6$. PL decay life time reveals the good intrinsic excitonic feature with less defect trappers [3]. Average life time for $Cs_2AgIn_{0.70}Bi_{0.30}Cl_6$ is 490 ns which is least among all other $Cs_2AgIn_{(1-x)}Bi_xCl_6$ doping. Thermogravimetric analysis (TGA) result reveals thermal stability of $Cs_2AgIn_{0.30}Bi_{0.70}Cl_6$ for the high-temperature 506°C. The Bi doping can decrease the band gap, restrict defect states, enhance PL and improve stability; these good performances make $Cs_2AgIn_{(1-x)}Bi_xCl_6$ more suitable for optoelectronic properties.

4:20pm **EM+2D+AN+MI+MP+NS-TuA7 Optimized (Quantum) Photonics**, ***Jelena Vuckovic,*** Stanford University **INVITED**

Photonics has numerous applications ranging from optical interconnects, classical and quantum computing, to sensing (such as LIDAR and AR), and imaging. However, the state of the art photonics is bulky, inefficient, sensitive to environment, lossy, and its performance is severely degraded in real-world environment as opposed to ideal laboratory conditions, which has prevented from using it in many practical applications. Therefore, it is clear that new approaches for implementing photonics are crucial.

We have recently developed a computational approach to inverse-design photonics based on desired performance, with fabrication constraints and structure robustness incorporated in design process [1,2]. Our approach performs physics guided search through the full parameter space until the optimal solution is reached. Resulting device designs are non-intuitive (see Figure), but are fabricable using standard techniques, resistant to temperature variations of hundreds of degrees, typical fabrication errors, and they outperform state of the art counterparts by many orders of magnitude in footprint, efficiency and stability. This is completely different from conventional approach to design photonics, which is almost always performed by brute-force or intuition-guided tuning of a few parameters of known structures, until satisfactory performance is achieved, and which almost always leads to sub-optimal designs.

Apart from integrated photonics, our approach is also applicable to any other optical and quantum optical devices and systems. In recent years, color centers in diamond and silicon carbide (SiC) have emerged as a possible platform for implementation of quantum circuits [3,4]. We demonstrate how such quantum hardware can also be optimized to be robust, efficient, and scalable.

References

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[3] J.L. Zhang et al, Nano Letters 18 (2), 1360-1365 (2018)

[4] M. Radulaski et al, Nano Letters 17 (3), 1782-1786 (2017)

5:00pm **EM+2D+AN+MI+MP+NS-TuA9 Optical Properties of Single Silicon Vacancies in 4H-SiC**, *H.B. Banks,* National Research Council Postdoc residing at the Naval Research Laboratory*; O. Soykal,* Sotera Defense Solutions, Inc, residing at the Naval Research Laboratory*; S.P. Pavunny, R.L. Myers-Ward, D.K. Gaskill,* ***Samuel Carter,*** U.S. Naval Research Laboratory

Defects in wide bandgap materials have generated substantial interest as promising systems for quantum information and quantum sensing due to bright, stable optical emission that is often coupled to long-lived spin states. One promising defect system is the silicon monovacancy in SiC (V_{Si}), which has a spin-3/2 ground state that can be optically polarized and maintain long spin coherence times even at room temperature. SiC is an attractive material in terms of mature growth and fabrication technology and also has a low natural abundance of nuclear spins, which reduces spin dephasing. While significant work has been performed to study the spin properties of V_{Si} for ensembles and even single defects, the optical properties and their connection to the spin system are less developed. Here we report on high resolution optical spectroscopy of single V_{Si} defects, specifically V2 defects, at low temperatures. Using laser excitation spectroscopy, the zero phonon line (ZPL) transitions corresponding to the m_s=±1/2 and m_s=±3/2 spin states are resolved, with a linewidth down to 70 MHz and a splitting of 1 GHz. While there is significant variation in the transition energies from one defect to another, the splitting of these lines is very uniform. We also find that emission from the V2 defect under resonant excitation of these lines rapidly decays on two very different timescales. Slow decay on a 10 ms timescale is attributed to photoionization of V_{Si} and can be prevented by periodically exciting the defect with a second laser at 745 nm. Fast decay on a μs or shorter time scale occurs due to a combination of intersystem crossing and spin polarization of the ground state. A significant difference in the decay rates of the two transitions is observed, which gives rise to spin-dependent photoluminescence intensity and non-resonant optical spin polarization. These results further our understanding of the connection between the optical and spin properties of this defect system that are necessary to optically control and readout the spin system as well as to develop a spin-photon quantum interface.

5:20pm **EM+2D+AN+MI+MP+NS-TuA10 Photoluminescence Studies on Patterned Silicon Vacancy Defects in Li Ion Implanted 4H-SiC for Scalable Quantum Device Applications**, ***Shojan Pavunny,*** U. S. Naval Research Laboratory*; S.G. Carter, H.B. Banks, R.L. Myers-Ward, P. Klein,* U.S. Naval Research Laboratory*; E.S. Bielejec,* Sandia National Laboratories*; M.T. DeJarld, A.S. Bracker, E.R. Glaser, D.K. Gaskill,* U.S. Naval Research Laboratory

Recently, silicon vacancy defect centers (V_{Si}) in the CMOS compatible wide bandgap semiconductor SiC hexagonal polytypes have drawn great research interest for future applications in scalable quantum information and quantum sensing mainly due to their high electronic spin (S = 3/2) with a long coherence time at room temperature. Realization of future densely integrated quantum devices will greatly benefit from the ability to deterministically induce the desired V_{Si} density at the optimal location in the three-dimensional solid-state matrix with nanometer accuracy and excellent optical properties. With this motivation, we demonstrate targeted formation of arrays of V_{Si} ensembles as well as single defects in high-quality 4H-SiC epilayers by a direct, maskless focused ion beam implantation technique with a designed lateral separation of ~5 μm and a ~25 nm spot size. We have carried out high-resolution optical spectroscopy studies (E⊥c and E ∥c) on these arrays, in which lithium ions are implanted at doses varying from 10^{12} – 10^{15} Li/cm^2 at a fixed energy of 100 keV to a depth of ~400 nm from the surface. Photoluminescence intensity and defect conversion yield with dose, photostability, fluorescence saturation, and V_1:V_1' intensity evolutions with temperature and excitation power were investigated. Results obtained from temperature dependent photoluminescence studies can provide key insights in the design and fabrication of scalable and reproducible three dimensional SiC quantum hybrid devices including photonic crystal cavities.

5:40pm **EM+2D+AN+MI+MP+NS-TuA11 Processing of Cavities in SiC Material for Quantum Technologies**, ***Rachael Myers-Ward**, K. Hobart, K.M. Daniels, A.J. Giles, M.J. Tadjer, L.E. Luna, F.J. Kub, S.P. Pavunny, S.G. Carter, H.B. Banks, E.R. Glaser,* U.S. Naval Research Laboratory*; P.B. Klein,* Sotera Defense Solutions*; K. Qiao, Y. Kim, J. Kim,* Massachusetts Institute of Technology*; D.K. Gaskill,* U.S. Naval Research Laboratory

Silicon carbide is a material of interest for quantum computing and sensing applications owing to deep point defect centers with long spin coherence times (which characterizes the lifetime of the qubit), specifically the V_{Si} [1], divacancies [2] and nitrogen-vacancy centers [3]. These spin qubits have been isolated and coherently controlled, where V_{Si} have T_2 coherence times up to 100 µs [4] and divacancies to 1 ms [2], making these two defects of most interest to date. While the current spin coherence times have been shown to be as long as 1 ms, further improvements are needed to fully realize the potential of SiC for quantum applications. In this work, we create V_{Si} in epitaxial SiC and investigate fabricating the layers into microstructures suitable for using the V_{Si} photoluminescence (PL) emission. We have found 4H-SiC epitaxial layers grown under standard growth conditions and with varying doping densities from 10^{14} to 10^{18} cm^{-3} have no measureable V_{Si} present, as determined by confocal PL. To introduce V_{Si}, we used 2 MeV electron irradiation in doses ranging from 0.75 to 75 kGy. This results in V_{Si} PL ranging from single to ensemble emission within the confocal volume. Hence, we are able to tune the vacancy concentration.

In order to improve the indistinguishable photons from the V_{Si} and/or divacancies for real applications, photonic crystal cavities (PCC) are used to tune the emission energy [4]. Our PCC design consists of a planar array of cylindrical holes approximately 220 nm wide in a slab of SiC, ~300-500 nm thin having an area 50 x 50 μm^2, similar to [4]. To maximize the PCC quality factor, the slab should have a large index of refraction difference on the top and bottom; i.e., an air gap is desired under the slab. To achieve this goal, we have identified four fabrication methods to create the PCC. One of these techniques is to use remote epitaxy as an innovative approach which entails growing epitaxial graphene on a SiC substrate by means of Si sublimation. Silicon carbide is then grown on a monolayer of graphene to the desired film thickness [5]. This thin SiC layer is then transferred, facilitated by the weak van der Waal forces at the graphene/SiC substrate interface, to a substrate more amenable to cavity fabrication. All four fabrication methods will be presented in detail.

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6:00pm **EM+2D+AN+MI+MP+NS-TuA12 Investigation of Localized Electronic structures of PbSe Quantum Dot Superlattice on a Highly Oriented Pyrolytic Graphite (HOPG)**, ***Il Jo Kwak**, S. Ueda,* University of California at San Diego*; A. Abelson, C. Qian, M. Law,* University of California, Irvine*; A.C. Kummel,* University of California at San Diego

Lead-Chalcogenide quantum dots are of interest due to the facility of adjustment of their electrical and optical properties. Using a colloidal self-assembly technique, extended arrays of nanocrystal QDs superlattices can be generated. The quantum confinement within individual QDs in the superlattice is relaxed and delocalization of wave functions occurs due to coupling of the QDs. In the QD solids, bulk-like electronic bands with a bandwidth of 100~200 meV are expected to form which yield much higher carrier mobility and diffusion length compared to weakly-coupled QDs; however, the electronic properties of such highly ordered QD arrays are not fully understood. The local density of state of a highly ordered monolayer PdSe superlattice was investigated by low temperature scanning tunneling microscopy.

A monolayer of PbSe QDs was prepared using the Langmuir Schaefer deposition technique. First, oleate-capped PbSe QDs dispersed in hexane were drop casted onto diethylene glycol surface. After the hexane was evaporated, a (111) in-plane oriented polycrystalline FCC superlattice was formed on the diethylene glycol surface. NH_4SCN solution was applied onto the oleate-capped PbSe superlattice film. The injection of NH_4SCN initiates the ligand exchange and phase transformation from an FCC to a simple cubic structure superlattice. A monolayer QD superlattice was prepared on a HOPG substrate. Afterward, the HOPG sample was loaded into a commercial UHV scanning tunneling microscopy chamber with a base pressure of $1x10^{-10}$torr. The sample was annealed to remove hydrocarbons and ligands from the surface. The topography of the QDs was observed with a tungsten tip. The STM images were acquired in constant current mode.

STM imaging showed the PbSe QD monolayer had 4-fold symmetry with an average inter QD spacing of 7nm. It is also found the height fluctuation of the QDs was 1nm indicating size variation of the QDs and imperfect crystal structure of the superlattice. Scanning tunneling spectroscopy was performed to investigate the electronic structure of the PdSe QDs using a variable z-mode with an external lock-in amplifier in the bias range of -2 to 2V. Single site STS showed resonant peaks from molecular orbitals of QDs before the ligand exchange process; however, the peaks were not observed after the ligand exchange due to necking between the QDs in the superlattice. In addition, the size of band gap was decreased as increasing the number of nearest neighboring QDs due to necking between QDs. Layer 2 QDs showed more p-type behavior than layer 1 QDs possibly due to the band bending effect at the interface of HOPG and QD superlattice.

2D Materials Focus Topic
Room 201B - Session 2D+AM+EM+NS-WeM

Dopants, Defects, and Interfaces in 2D Materials

Moderator: Eric Pop, Stanford University

8:00am **2D+AM+EM+NS-WeM1 Carbon Doping of 2D Transition Metal Dichalcogenides by Plasma Enhanced CVD**, ***Yanfu Lu***, *F. Zhang, S. Sinnott, M. Terrones,* The Pennsylvania State University

Doping of 2D transition metal dichalcogenides has been discovered to be an effective way to tune the electronic structure and modify the lattice structure at the surface. The n-type and p-type doping of monolayer MoS_2/WS_2 heterostructures may enable the fabrication of field-effect transistors of ultra-low thickness. Plasma enhanced chemical vapor deposition provides a stable and controllable approach for introducing carbon dopants to monolayer WS_2. Photoluminescence measurement indicates that the band gap of C-doped WS_2 decreases by 0.17 eV. Corresponding first principles calculations provide the correlation between the position and chemical saturation of the carbon dopants and the electronic structure of the system. To verify covalently bonded dopants, we use Raman spectroscopy, X-ray photoelectron spectroscopy, and scanning transmission electron microscopy to examine the pristine sample and carbon-doped samples. Subsequent I-V characteristics measurements prove p-type doping and the energy band diagram. Finally, the mechanism associated with and, more importantly, the structure-property relationship of chalcogen doping are analyzed. The resulting new insights of transition metal dichalcogenide-based heterostructures and alloys are discussed.

8:20am **2D+AM+EM+NS-WeM2 Methoxy Formation Induced Defects on MoS_2***, ***Duy Le***, University of Central Florida*; P. Evans,* University of Nebraska - Lincoln*; Z. Hooshmand,* University of Central Florida*; T.B. Rawal,* Oak Ridge National Laboratory*; L. Bartels,* University of California, Riverside*; P.A. Dowben,* University of Nebraska-Lincoln*; T.S. Rahman,* University of Central Florida

Defects are known to play an important role in determining the chemical properties of otherwise inert MoS_2 basal plane. Here we report our joint experimental and theoretical study of the adsorption and reaction of methanol on the MoS_2 basal plane to determine the factors that control system reactivity. We find that exposure of the MoS_2 basal plane to methanol leads to the formation of adsorbed methoxy and coincides with sulfur vacancy generation and that the methoxy moieties bind to molybdenum, not sulfur, while some adsorbed methanol is readily desorbed near or slightly above room temperature. Our calculations also suggest that the dissociation of methanol via O–H bond scission occurs at the defect site (sulfur vacancy), followed subsequently by formation of a weakly bound H_2S species that promptly desorbs from the surface with creation of a new sulfur vacancy, in great agreement with photoluminescence and scanning tunneling microscopy data that show clear evidence of the sulfur vacancy creation on the MoS_2 surface, after exposure to methanol [1].

[1] P. Evans et al, J. Phys. Chem. C (2018). DOI: 10.1021/acs.jpcc.8b02053

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

8:40am **2D+AM+EM+NS-WeM3 Defect Engineering of 2D Materials for Advanced Electronic Devices**, ***Gwan-Hyoung Lee***, Yonsei University, Republic of Korea **INVITED**

Two-dimensional (2D) materials have brought a great deal of excitement to nanoscience community with their attractive and unique properties. Such excellent characteristics have triggered highly active researches on 2D material-based electronic devices. New physics observed only in 2D semiconductors allow for development of new-concept devices. Assembly of 2D blocks for van der Waals heterostructures also provide a big playground for engineers and physicists to investigate unprecedented properties of 2D materials and fabricate multi-functional electronic devices. However, atomically thin 2D materials, such as graphene and transition metal dichalcogenides (TMDs), have only two surfaces at top and bottom without a bulk so that they are very sensitive to environment. In other words, properties of 2D materials can be altered easily by surface modification. In this talk, I will show novel approach to fabricate high performance 2D electronic devices by utilizing various surface treatments, such as fluorination and hydrogenation of graphene and layer-by-layer oxidation of MoS_2. When different types of defects, such as sp^3 bonds and vacancies, are induced on the surface of graphene, the electrical properties of graphene can be tuned. With mild plasma treatment, MoS_2 can be oxidized layer-by-layer and monolayer MoS_2 can be fabricated from the multilayer MoS_2. These surface treatment techniques can be used for fabrication of high performance graphene devices and MoS_2 optoelectronic devices. Defect engineering of 2D materials holds a great promise in engineering the 2D materials and fabricating advanced electronic devices of 2D materials.

9:20am **2D+AM+EM+NS-WeM5 Modeling Defects and Electron-electron Interactions in Low-dimensional Materials**, ***Daniel Gunlycke***, *C.E. Ekuma,* U.S. Naval Research Laboratory

While each nanoscale structure in a low-dimensional material can exhibit a variety of properties, the odds are that it will be (1) sensitive to defects and (2) strongly influenced by electron-electron interactions. The ratio of defect sites to pristine sites naturally increases, as structures become smaller. Electron localization can furthermore dramatically magnify the role of defects. In low-dimensional materials, dielectric screening is generally less effective, reducing the tendency for electronic interactions to become uniform across the sites in the materials. Despite the importance of both defects and electron-electron interactions, the properties of low-dimensional materials are often investigated in the absence of one or the other. This not only creates uncertainty over the predictions but could entirely miss certain physical phenomena, including insulator-to-metal transitions. In this presentation, we will discuss a general first-principles-based approach to explore realistic low-dimensional structures that explicitly accounts for both defects and electron-electron interactions [1]. It is based around a generalized Anderson Hamiltonian and applies density functional theory, as well as dynamical mean-field theory. We will also present electronic and optical properties of two-dimensional materials obtained using our method and discuss the potential for using defect engineering for improved solar cell performance.

[1] C. E. Ekuma, V. Dobrosavljevic, and D. Gunlycke, *Physical Review Letters* **118**, 106404 (2017)

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

9:40am **2D+AM+EM+NS-WeM6 Post-Synthesis Modifications of Two-Dimensional $MoSe_2$ or $MoTe_2$ by Incorporation of Excess Metal Atoms into the Crystal Structure**, ***Paula Mariel Coelho***, University of South Florida*; H. Komsa,* Aalto University, Finland*; H. Coy Diaz, Y. Ma,* University of South Florida*; A.V. Krasheninnikov,* Institute of Ion Beam Physics and Materials Research, Germany*; M. Batzill,* University of South Florida

Modifications of $MoSe_2$ and $MoTe_2$ with metallic mirror twin grain boundaries (MTB) in films grown by molecular beam epitaxy have been previously reported [1,2]. The goal of the study presented here has been to understand the formation-mechanism of MTB networks and apply this gained knowledge for controlled modifications of these 2D materials. In a combined scanning tunneling microscopy and density functional theory approach we demonstrate that excess Mo can easily diffuse into the pristine $MoSe_2$ or $MoTe_2$ (but not into MoS_2) layer and cause crystal modifications into Mo-rich twin grain boundaries. Vapor deposited Mo atoms are first incorporated by diffusing into interstitial (or split-interstitial) sites. Then, further Mo-atoms incorporate into the crystal structure to form triangular, Mo-rich grain boundary loops. Only after a critical density of MTBs is reached, Mo is no-longer absorbed by the 2D-crystal sheet and Mo-clusters start to form at the surface. The energetics and barriers for Mo-incorporation is calculated by DFT and shows that the formation of twin grain boundaries in the presence of excess Mo is favorable for $MoTe_2$ and $MoSe_2$, but not for MoS_2 - in agreement with the experiment. The achievable dense networks of MTBs constitute a new Mo-rich metallic phase that may be used for controlled electric contacts or creation of active sites in electro-catalysis [4] and thus adding new functionalities into transition metal dichalcogenide-based materials and devices. Moreover, DFT simulations suggest that this mechanism for incorporation of transition metals is not limited to Mo. This enables modification of the materials properties by heteroatom dopants and initial experimental work demonstrates the incorporation of both Ti and V. V-interstitials in $MoTe_2$ are predicted to have a magnetic moment and magnetic hysteresis curves indicate the induction of ferromagnetism in $MoTe_2$ by doping the material with less than 1% of V interstitials.

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[3] Ma Y. et al. (2017) Angle resolved photoemission spectroscopy reveals spin charge separation in metallic MoSe2 grain boundary. Nat. Commun. 8, 14231.

[4] Tomasz Kosmala et al. (2018) Metallic Twin Boundaries Boost the Hydrogen Evolution Reaction on the Basal Plane of Molybdenum Selenotellurides. *Adv. Energy Mater.* 2018, 1800031.

11:00am **2D+AM+EM+NS-WeM10 Dry Cleaning and Doping of MX_2 for Contact Engineering**, ***Daniil Marinov***, IMEC, Belgium; *J. Ludwig,* IMEC & KU Leuven, Belgium; *D. Chiappe,* IMEC, Belgium; *E. Voronina, T. Rakhimova,* Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University; *J.-F. de Marneffe, I. Asselberghs,* IMEC, Belgium; *S. De Gendt,* IMEC, KU Leuven, Belgium

Two-dimensional transition metal dichalcogenides (e.g. MoS_2, WS_2) are promising materials for a number of electronic and optoelectronic applications. Wafer-scale integration of these materials into sophisticated devices requires atomic-scale control of the processing steps such as deposition, etch, clean and doping. Reduction of the contact resistance is a major roadblock towards demonstration of high-performance devices. Significant Schottky barrier at the metal-MX_2 interface as well as surface contamination (e.g. by polymer residues) are the main factors contributing to the high contact resistance in fabricated MX_2 devices. In this study, a fully dry cleaning and doping technique is developed with a particular focus on contact engineering.

We demonstrate that a remote H_2 plasma is efficient for removal of organic residues from MX_2 surfaces. However, sulfur can be also stripped from the topmost layer by reactive H atoms. The main challenge is thus to precisely control the sulfur loss while maintaining the cleaning efficiency. At high substrate temperature, a 200 nm PMMA layer can be fully removed selectively to a single layer of WS_2 without damaging the 2D material (as confirmed by photoluminescence measurements). At low substrate temperatures significant S-vacancy formation was observed. Surface temperature is therefore the key parameter for controlling the reactivity of H atoms on WS_2.

Controllable formation of sulfur vacancies opens routes for substitutional doping. After H_2 plasma strip, WS_2 and MoS_2 samples were exposed to a flow of molecular gases (Cl_2, CO, OCS) without igniting the plasma. It is shown that Cl_2 and OCS can react with H_2 plasma treated MX_2 forming stable surface groups. Ex-situ conductive AFM measurements confirm that molecular doping prevents the loss of conductivity (that is observed after H_2 plasma alone). Moreover, OCS and Cl_2 exposure enhances electrical current injection in the material through grain boundaries and edges. The latter effect is beneficial for contact resistance reduction on MX_2.

To gain a deeper insight in the observed surface phenomena, DFT simulation of the interaction of atomic (H, Cl, F) and molecular (OCS, Cl_2) species with MX_2 surface was performed. S-vacancy creation by atomic hydrogen via formation of gas phase H_2S was observed in simulations, in qualitative agreement with the experiments. Moreover, dissociative adsorption of Cl_2 and OCS in S-vacancy sites is predicted by the DFT model.

Dr D. Marinov has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 752164.

11:20am **2D+AM+EM+NS-WeM11 Deep Learning for Atomically-Resolved Scanning Transmission Electron Microscopy Experiments on 2D Materials**, ***Maxim Ziatdinov***, *S.V. Kalinin,* Oak Ridge National Laboratory

Understanding fundamental atomic-scale mechanisms behind solid state reactions and phase transformations is critical for optimizing functional properties of technologically relevant materials. Recent advances in scanning transmission electron microscopy (STEM) have allowed to visualize dynamic processes in solid state systems, induced by thermal or chemical stimuli or electron beam, on the level of individual atoms and single atomic defects. However, while there have been multiple STEM studies on materials structure evolution, the materials-specific knowledge on the kinetics and thermodynamics of these processes and atomic potentials is almost non-existent, which is mainly due to the inherent limitations of the current (semi-)manual image analysis techniques. Here we demonstrate an approach based on deep convolutional neural networks for automated analysis of dynamic STEM data from 2-dimensional materials, such as monolayer WS_2, under e-beam irradiation. Our approach allows to create a library of atomic defects, explore subtle atomic distortions around the defects of interest and map chemical transformation pathways on the atomic level. We specifically show how the developed framework can be used for extracting diffusion parameters of sulfur vacancies in WS_2 and for studying transformation pathways for Mo-S complexes, including detailed transition probabilities.

11:40am **2D+AM+EM+NS-WeM12 Magnetic Doping in 2D MBE-grown-$MoSe_2$/graphene Heterostructures Studied by Photoelectron Spectroscopy and Band Structure Imaging**, ***Maxime Gay***, *O.J. Renault,* CEA-LETI, France; *MT. Dau, C. Vergnaud, M. Jamet,* CEA-INAC-SPINTEC, France

2D TMDCs present a unique combination of electronic and mechanical properties such as a direct bandgap, strong spin-orbit coupling and K-valley inequivalence, with an atomic-scale thickness [1]. Introducing magnetic phases into these materials opens exciting perspectives towards spin control in magnetic tunnel junctions. To date, magnetism in 2D systems was mostly studied by theoretical calculations. Within the diluted magnetic semiconductors model, transition metal atoms from the monolayer are substituted by a few Mn, Fe or Co atoms [2-4].

Our study focuses on Mn-doped-$MoSe_2$ monolayers, grown by molecular beam epitaxy on graphene, and characterized by photoemission techniques (XPS, kPEEM) coupled with observations at different scales (DRX, TEM). Before doping, we found that the in-plane lattices of graphene and $MoSe_2$ are aligned with each other and that a bandgap opens in the graphene around the Fermi level [5-6]. After Mn doping, the obtained Mn insertion is measured up to 15% by XPS. The influence of Mn doping on the band structure of $MoSe_2$/graphene heterostructure will be presented and discussed.

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Nanometer-scale Science and Technology Division
Room 203A - Session NS+2D+AN+MN+MP+SE-WeM

Micro, Nano and Opto Mechanics

Moderators: Robert Ilic, National Institute of Standards and Technology, Alokik Kanwal, NIST Center for Nanoscale Science and Technology

8:20am **NS+2D+AN+MN+MP+SE-WeM2 The Collective Behavior of Large Ensembles of Coupled MEMS Cantilevers with Varying Natural Frequencies**, ***Christopher Wallin***, National Institute of Standards and Technology, Center for Nanoscale Science and Technology; *N. Dick,* Tel Aviv University, Israel; *R. De Alba, D.A. Westly,* National Institute of Standards and Technology, Center for Nanoscale Science and Technology; *S. Grutzik,* Sandia National Laboratories; *A.T. Zehnder, R.H. Rand,* Cornell University; *V.A. Aksyuk,* National Institute of Standards and Technology, Center for Nanoscale Science and Technology; *S. Krylov,* Tel Aviv University, Israel; *B.R. Ilic,* National Institute of Standards and Technology, Center for Nanoscale Science and Technology

The collective behavior of nonlinear, coupled micro- and nano-electromechanical (M/NEMS) resonators has been shown to exhibit a host of nontrivial dynamics including abrupt pattern switching, multistability, hysteresis, intrinsically localized modes, and synchronization. Additionally, M/NEMS resonator arrays are extremely responsive to environmental perturbations making them excellent candidates for sensing applications when operated linearly. With our work, we investigate the collective dynamics of coplanar interdigitated arrays of prismatic microcantilevers operating in both the nonlinear and linear regimes.

Two opposing, partially interdigitated cantilever arrays with 100 cantilevers apiece were fabricated using a silicon–on–insulator wafer. The device consists of a unique geometry in which each array has cantilever lengths expanding linearly across the device in opposite directions giving a distribution of natural frequencies. The arrays were engineered to allow for large scale, nonlinear out-of-plane beam deflections through the removal of the entire silicon handle layer beneath the active array area.

For sufficiently large drive amplitudes, the resonators begin oscillating via combination parametric resonance (CPR) across the entire array. The CPR

driven oscillations occur across a broad frequency band. The tunable coupling between nearest-neighbor cantilevers through fringing electrostatic fields provides a mechanism to vary the CPR response. Due to the sizable deflections, the device's nonlinearities are apparent including hysteresis effects. Our experimental results are supported and expanded by the development of a reduced order model based on the Galerkin decomposition which generates the leading features of our data including the CPR band.

When operating in the linear regime, the natural modes of the array have localized characteristics whereby a limited number of beams oscillate at each of the natural mode frequencies. Operating the device at higher harmonics increases mode separation as the propagation bands stretch. The distinct resonant peak separation coupled with the spatially confined modal response make higher harmonic operation of tailored, variable length cantilever arrays well suited for a variety of resonant based sensing applications.

8:40am **NS+2D+AN+MN+MP+SE-WeM3 Piezoelectric Optomechanical Systems**, ***Krishna Coimbatore Balram,*** University of Bristol, UK **INVITED**

Nanoscale optomechanical systems, which rely on the strong interactions between co-localised optical and mechanical modes in nanoscale cavities, have been explored for a wide variety of applications ranging from sensing to signal transduction [Aspelmeyer et al., Rev. Mod. Phys. (2014)]. In this talk, I will discuss piezoelectric optomechanical platforms for efficient signal transduction between the radio frequency (RF) and optical domain. We use GaAs as our model platform (Balram et al., Optica (2014), Nature Photonics (2016), Phys. Rev. Applied (2017)) and discuss some of the research opportunities and challenges in this field, especially as we move towards higher mechanical frequencies (> 10 GHz).

9:20am **NS+2D+AN+MN+MP+SE-WeM5 Absolute Deflection Measurements in a MEMS/NEMS Fabry-Perot Interferometry System**, ***Roberto De Alba****, C.B. Wallin, G. Holland,* National Institute of Standards and Technology*; S. Krylov,* Tel Aviv University, Israel*; B.R. Ilic,* National Institute of Standards and Technology

Micro- and nano-electromechanical systems (MEMS/NEMS) are among the most sensitive devices for detection of ultra-weak forces, masses, and displacements. The small scale of these structures affords them very high frequencies (MHz to GHz), high quality factors, rich nonlinear phenomena, and many other beneficial traits that make them ideal as sensors and testbeds of fundamental physics. Fabry-Perot laser interferometry is a widespread and robust technique for probing MEMS/NEMS devices because it is non-invasive and provides exceptional motion sensitivity (≈ 1 pm/$Hz^{1/2}$) from DC to roughly 100 MHz. This technique utilizes the silicon substrate beneath the MEMS/NEMS device as a static reference mirror; doing so provides common-mode noise rejection in contrast to interferometers that use an external reference mirror. Furthermore, this technique is compatible with a wide range of MEMS/NEMS materials, from common insulators and conductors to graphene and other atomically-thin membranes.

Despite the many strengths of this experimental technique, it suffers from two main drawbacks. Firstly, the measured signal becomes highly nonlinear for device displacements larger than λ/4, where λ is the laser wavelength. Secondly, because the silicon backplane is immovable, there is no simple or established technique for calibrating device motion. As such, published results utilizing this setup typically report deflection in "arbitrary units." In this work, we focus on fully characterizing the nonlinear aspects of a MEMS/NEMS Fabry-Perot interferometer and developing a generalized approach to calibrate device motion based the wavelength of light. We will demonstrate how to quickly and accurately determine both static and dynamic MEMS/NEMS deflection by measuring reflected laser power in the time domain. We will further show how a single calibration (made in the large-amplitude regime) can be applied to subsequent measurements taken at lower amplitudes as well as to measurements taken in the frequency domain (e.g. by a lock-in amplifier). Lastly, we will demonstrate the capability of imaging the first three vibrational modes of a MEMS cantilever by using a scanning laser.

9:40am **NS+2D+AN+MN+MP+SE-WeM6 Silicon on Insulator Electrostatically Actuated Bistable Cantilevers for Resonant Displacement/Acceleration Sensing**, *O. HaLevy, E. Benjamin, N. Krakover, Y. Kessler,* ***Slava Krylov,*** Tel Aviv University, Israel

Resonant accelerometers incorporating vibrating beams demonstrate higher sensitivity and better robustness when compared to their statically operated counterparts. Electrostatic softening of the beams electrostatically coupled to the proof mass allows to enhance sensitivity of the resonant accelerometers. The displacement of the proof mass affects the gap between the mass and the beam and results in the beam's frequency change, which is maximal in the vicinity of the critical limit points of the voltage-deflection curve. The use of the snap-through buckling for this purpose is attractive since it is fully reversible and does not involve contact. While double-clamped curved bistable beams designed to demonstrate snap-through behavior can serve as resonant acceleration sensors [1], they suffer from high sensitivity to temperature and residual stress.

In this work we report on a design and fabrication of an electrostatically actuated bistable resonant cantilever [2], which demonstrates low sensitivity to the temperature and to the residual stress. The concept is based on the tailoring of the actuating force in such a way that the beam in its initial "as fabricated" configuration is positioned in the vicinity of the critical point. This is achieved by designing the actuating electrodes to be significantly thicker that the beam. Our reduced order (RO) Galerkin and coupled finite elements (FE) models results show that the frequency to deflection sensitivity of the L = 150 μm long, h = 16 μm wide and d = 1 μm thick cantilever can reach 20 Hz/nm. This is equivalent to the frequency to acceleration sensitivity of 388 Hz/g, obtained for the case of a 4 mm × 4 mm × 20 μm proof mass.

While the model results are promising, fabrication of the device incorporating the beams and the electrodes of the different thicknesses is challenging. We demonstrate fabrication of the 50 μm thick electrodes and ≈6 μm thick cantilevers from the same device layer of a Silicon on Insulator (SOI) wafer. Two-stage deep reactive ion etching (DRIE) process was used for an initial patterning of the electrodes and of the cantilever and for the thinning of the beams. We discuss the details of the fabrication process and preliminary experimental results.

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11:00am **NS+2D+AN+MN+MP+SE-WeM10 Electron-Photon-Phonon Hybrid Systems Based on Compound Semiconductor Mechanical Resonators**, ***Hiroshi Yamaguchi,*** NTT Basic Research Laboratories, Nippon Telegraph and Telephone Corporation, Japan **INVITED**

The use of compound semiconductor heterostructures as the elastic materials in the fabrication of micro/nanomechanical resonators has advantages, such like the improvement of mechanical properties through strain engineering, optomechanical transduction through carrier-mediated coupling, and piezoelectrically controllable nonlinearity [1]. The hybrid properties play the essential role in the operation where the different excitations of phonons, photons, and electrons are mutually interacted. In this invited talk, I will review our recent activities studying the electronic [2], photonic [3], and phononic [4] functions in GaAs-based mechanical resonators.

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11:40am **NS+2D+AN+MN+MP+SE-WeM12 Size Dependent Mechanics of Elastomers**, ***Le Li,*** *N. Alsharif, K.A. Brown,* Boston University

Elastomers are fascinating materials owing to the fact that their mechanical properties are dictated by entropy. Due to their low modulus, chemical compatibility, and ease of processing, they are widely applied in fields from soft lithography to medical devices. While it is well accepted that they exhibit fascinating size-dependent mechanical properties when confined to thin films, the structure-property relationships that govern confined elastomers are difficult to unambiguously determine due to the mechanical influence of rigid support structures and unavoidable contributions from adhesion. As a result, a consensus regarding the moduli of elastomeric thin films has not emerged. Here, we present a combined computational and experimental approach to measure the true mechanical properties of thin elastomer films. First, we utilize extensive finite element simulations to

determine a correction to the Hertzian contact model that depends upon a dimensionless film thickness and the polymer Poisson's ratio. In order to verify this correction, films composed of three different thermoplastics were studied using an atomic force microscopy (AFM) nanoindenting. Interestingly, all three were observed to soften when confined to films thinner than 100 nm, in agreement with literature reports of buckling experiments. To explore softer elastomeric materials that exhibit categorically different behavior, we extended this correction to the Johnson-Kendall-Roberts (JKR) model that considers adhesion in contact mechanics. Elastomer thin films with different crosslink densities were studied using AFM nanoindentation and finite element simulation to determine their moduli. We observed a drastic stiffening on all elastomeric films when they were confined to sub-micrometer thicknesses. More importantly, modulus of all sub-100 nm elastomer films converges to the same trend regardless of bulk crosslink density. We present a hypothesized molecular model explaining this behavior. These results shed new light on the nanomechanics of elastomers and provide a general process for exploring size-dependent mechanics in polymers.

2D Materials Focus Topic
Room 201B - Session 2D+MN+NS+SS-WeA

IoT Session: Surface Chemistry, Functionalization, Bio and Sensor Applications

Moderator: Daniel Walkup, National Institute of Standards and Technology (NIST)/ University of Maryland, College Park

2:20pm **2D+MN+NS+SS-WeA1 Impact of Hydrogen on Graphene-based Materials: Atomistic Modeling and Simulation of HRSTEM Images**, *C. Guedj,* Univ. Grenoble Alpes, CEA, LETI, France*; L. Jaillet, F. Rousse,* ***Stéphane Redon,*** Univ. Grenoble Alpes, CNRS, INRIA, Grenoble INP*, LJK, France

The hydrogen energy transition is highly probable, because hydrogen is the most abundant element in the universe and represents an ideal "green" source of energy. Meanwhile, the safe hydrogen production and storage remains a major challenge still in progress. Potential production and storage materials include graphene. In terms of electronic and optoelectronic applications, hydrogen can tune the bandgap of graphene [1]. Hydrogen also plays a major role during the Chemical Vapour Decomposition (CVD) growth of graphene [2]. Hence, hydrogenated graphene-based materials are potentially relevant for various technological applications.

To understand and optimize the device efficiency and the interface engineering, it is advantageous to perform advanced nanocharacterizations, linked to numerical modelling and simulations. This task is particularly difficult, because hydrogen is labile and prone to rapid reorganization. This structural evolution may be monitored with transmission electron microscopy (TEM) techniques [3,4,5], but in spite of significant progresses, the direct detection of hydrogen with High Resolution Scanning Transmission Electron Microscopy (HRSTEM) or energy-loss spectroscopy still remains a serious challenge.

We investigate here the interaction of hydrogen with graphene using the Brenner module of the SAMSON software platform https://www.samson-connect.net and we propose an original methodology to characterize its structural arrangement at the atomic scale by simulating HRSTEM images to interpret experimental results. In particular, we compare the effect of hydrogen on dark field (DF), bright field (BF), high-angle annular dark filed (HAADF) and annular bright field (ABF) images, to estimate the best technique suited to hydrogen detection.

In addition, we present the effect of carbon vacancies and adatoms on the stability of hydrogen coverage, associated to the HRSTEM signatures of the most stable configurations. These results provide the necessary building blocks to analyze the structure and energetics of hydrogenated graphene-based materials at the atomic scale.

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2:40pm **2D+MN+NS+SS-WeA2 High Density H2 and He Plasmas: Can They be used to Treat Graphene?**, ***Hasan-Al Mehedi,*** Laboratoire des Technologies de la Microélectronique, CNRS-UJF, France*; D. Ferrah,* Cea, Leti, Minatec, France*; J. Dubois, C. Petit-Etienne,* Laboratoire des Technologies de la Microélectronique, CNRS-UJF*; H. Okuno,* Cea, Inac/sp2m/lemma*; V. Bouchiat,* Institut Néel, CNRS-UJF-INP*; O.J. Renault,* CEA/LETI-University Grenoble Alpes, France*; G. Cunge,* Laboratoire des Technologies de la Microélectronique, CNRS-UJF, France

Since graphene and other 2D materials have no bulk, a major issue is their sensitivity to surface contaminations, and the development of cleaning processes is mandatory. High density plasmas are attractive to treat (clean, dope, pattern) 2D materials because they are a mature industrial technology adapted to large area wafer. However, in these plasmas the substrate is bombarded by a high flux of both thermal radicals and reactive ions with typical energy above 10 eV, which can easily damage atomic layer thin materials. We have investigated systematically the interaction of H2 and He inductively coupled plasmas (ICP) with graphene in industrial reactors. We report a specific issue associated with the use of H2 plasma: they etch the inner part of plasma reactor walls, thus releasing impurities in the plasma, most notably O atoms that etch graphene and Si atoms which stick on it. The presence of parasitic oxygen presumably explains the discrepancies found in the literature regarding the impact of reactive plasmas on graphene damages. To get rid of this issue we propose to use a fluorinated aluminum chamber. In this case, fluorine atoms which are shown to be harmless to graphene are the only impurity in the plasma. Under such conditions H2 ICP plasma is shown to clean graphene without damages if the ion energy is kept below about 15 eV.

3:00pm **2D+MN+NS+SS-WeA3 Novel Binder-free Ag@Ni(OH)$_2$ over Graphene/Ni Foam and Glucose Sensing**, ***Tong-Hyun Kang****, J.-S. Yu,* DGIST, Republic of Korea

Graphene combining with metal nanoparticles or other compounds is widely recognized to be a viable strategy to assemble high-activity catalysts.Unique properties of high conductivity and transparency, 2D morphology, and high stability in acid and alkaline solutions make graphene an excellent electron transfer medium on the interface of graphene/active materials as catalysts.Among them, graphene/metal nanoparticle (G/MNP) composites have been attracting more interest because of remarkably enhanced catalytic property, which is ascribed to a synergic effect from the interface of graphene and active sites. In general, reducing agents and electrodeposition methodshave been employed to *in-situ* reduce metal ions such as Au^{3+}, Pt^{4+}, Ag^{+}, and Cu^{2+} (M^{x+}) to MNPs on the graphene to form G/MNP composites.In this study, graphene is grown on nickel foam (NF) by chemical vapor deposition (CVD), which is directly used for MNP deposition. Different from bare NF, special phenomenon is observed that the graphene-coated nickel foam (GNF) composite can greatly speed up the electrodeless reduction of M^{x+} ions on the surface of the graphene. Interestingly, the MNP deposition and Ni(OH)$_2$ nanosheet assembly simultaneously occur on the GNF. Binder-free Ni(OH)$_2$-wrapped Ag hybrid developed on the GNF (Ag@Ni(OH)$_2$-GNF) is found to serve as an efficient electrochemical sensor because of its unique structure. A low detection limit of 0.3 μM and high sensitivity are achieved for the glucose detection, which confirms that the hierarchical electrode structure of Ag@Ni(OH)$_2$-GNF composite is highly effective to have extensive applications.

3:20pm **2D+MN+NS+SS-WeA4 Surface Modification and Magnetization of Carbon Based Nanostructures**, ***Rina Tannenbaum,*** University of Stony Brook*; I.T. Kim,* Gachon University, Korea*; S. Sharma,* University of Stony Brook

We describe here a novel synthesis for the facile decoration of carbon nanomaterials (CNM) with monodisperse γ-Fe_2O_3 magnetic nanoparticles. These procedures were developed for multi-walled carbon nanotubes (MWNTs), reduce graphene (rGO) and reduced graphene nanoroses (rGO-roses). The decoration of these carbon nanomaterials with γ-Fe_2O_3 induces the magnetization of these structures and opens up the potential for their use in novel applications.

CNM/γ-Fe_2O_3 magnetic nanostructures were fabricated through a modified sol-gel process using ferric nitrate nonahydrate, $Fe(NO_3)_3{\cdot}9H_2O$ as a starting material. Nucleation sites for the iron oxide were generated at the CNM surface due to the electrostatic interaction between Fe (III) ions and the carboxylate surface groups of acid-treated CNMs. The occurrence of gelation was inhibited by the addition of the NaDDBS surfactant, before the addition of propylene oxide, which is a gel promoter. The surfactant interfered in the growth stage of the iron oxide nanoparticles (gel phase) through to the coordinaton of the NaDDBS molecules to the iron (III) centers due to the attraction between the negatively-charged hydrophilic head of the surfactant and the positively-charged iron. The rGO-roses were further fabricated from decorated rGO via a novel emulsion process.

Various characterization methods were used to confirm the formation of well-defined maghemite nanoparticles, and show that they were tethered to the walls of the CNMs. The tethered γ-Fe_2O_3 nanoparticles imparted magnetic characteristics to the CNMs, which in turn, became superparamagnetic. The magnetic carbon nanotubes and magnetic rGO were introduced into a polymer matrix [#] and were oriented parallel to the direction of an externally-applied magnetic field. The anisotropic nanocomposites were then used as anodes in lithium ion batteries. The magnetic rGO-roses were used as nuclear magnetic resonance contrast material.

4:20pm **2D+MN+NS+SS-WeA7 Chemical Modification of Graphene and Carbon Nano Tubes as viewed by XPS and NEXAFS Spectroscopies underpinned by DFT Spectra Simulation**, *C. Ehlert, E. Donskyi,* Bundesanstalt für Materialforschung und -prüfung (BAM), Germany*; P.L. Girard-Lauriault,* McGill University, Canada*; R. Illgen,* Bundesanstalt für Materialforschung und -prüfung (BAM), Germany*; A. Lippitz,* Bundesanstalt für Materialforschung und -prüfung (BAM)*; R. Haag, M. Adeli,* Freie Universität Berlin, Germany*;* ***Wolfgang Unger****,* Bundesanstalt für Materialforschung und -prüfung (BAM), Germany

Graphene is a two-dimensional carbon network with unique properties. However, its low solubility, poor reactivity and the limited accessibility of a well-defined basal plane are major challenges for applications. An ideal method to overcome these problems is the covalent attachment of functional molecules to its surface which enable further reactive modifications for specific applications. There are several technologies for surface functionalization of graphene and related CNT materials. To get control on the functionalization process and to optimize the performance of the modified surfaces analytical tools for surface chemical characterization are required. X-ray absorption (NEXAFS) and photoelectron spectroscopy (XPS) have been identified to be rather powerful here [1-3]. Specifically, NEXAFS spectroscopy underpinned by quantum chemical spectrum simulations [4] is unique in a way to address changes of aromaticity and defect formation at the graphene surface during functionalization.

For relevant surface modification technologies, we present examples on how NEXAFS and XPS are fit for purpose. All presented modifications aim on the production of platforms for defined functional 2D nanomaterials, as for example multi-functional hybrid architectures. In detail we investigated:

- A wet chemical method for covalent functionalization of graphene sheets by a one-pot nitrene [2+1] cycloaddition reaction under mild conditions. Here a reaction between 2,4,6-trichloro-1,3,5-triazine and sodium azide with thermally reduced graphene oxide (TRGO) results in defined dichlorotriazine-functionalized graphene sheets.
- Graphene and carbon nanotube functionalized by Vacuum-Ultraviolet (VUV) induced photochemical or r.f. cw low pressure plasma processes to introduce amino, hydroxy or brominated functionalities.

To underpin finger-print information delivered by C K-edge NEXAFS we studied the effects of selected point and line defects as well as chemical modifications for a single graphene layer model by density functional theory based spectrum simulations.

Acknowledgement

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4:40pm **2D+MN+NS+SS-WeA8 Elastic Spongy Graphene-Functionalized Silicon Anode with Excellent Cycle Stability in Li battery**, ***Byong-June Lee****, J.-S. Yu,* DGIST, Republic of Korea

Graphite plays a prominent role as a typical anode material in the lithium ion batteries (LIBs) because of its high lithiation-dilithiation reversibility and low voltage window. Unfortunately, the capacity is limited to 372 mAh g^{-1}[1,2]. To search for materials with higher lithium storage capacity, a great number of investigations on metal oxides (or sulfides), Sn, P, and Si have been carried out in recent decades. Among these materials, silicon can make alloy with lithium in the form of $Li_{22}Si_5$ to deliver a highest theoretical gravimetric capacity of ~4200 mAh g^{-1}, and thus is considered to be one of the most promising anode materials for next generation LIB. It is worth mentioning that its quite low delithiation potential and high lithium storage capacity can provide a wide working voltage window and energy density, which enable promising potential application in electric vehicles. However, those advantages are seriously offset by a great challenge of large volume expansion during lithiation process and the resultant breakage of bulk silicon particles and solid electrolyte interface (SEI), which causes a serious damage to the electrode structure and thus gives rise to a fast decay of the specific capacity [3].

In this work, novel 3D spongy grapheme (SG)-functionalized silicon is for the first time demonstrated by chemical vapor deposition for a LIB anode, which can overcome the common silicon anode issues such as poor conductivity and volume expansion of Si as well as transfer of Li ion towards the Si. The elastic feature of graphene has excellent function to self-adaptively buffer the volume variation during charge-discharge process. In particular, different from traditional graphene or carbon shells (core-shell and yolk-shell), the spongy 3D graphene networks provide much improved unique functions with excellent long-cycle stability and rate capability. The Si@SG electrode exhibits excellent cycling performance with high reversible specific capacity [4]. A superior 95% capacity retention is achieved after 510 cycles. All the electrochemical performances get benefits from the well-designed functional SG shells, where interconnected nano-graphene structure not only guarantees a high conductive network but also provides more free paths for excellent mass transfer in addition to self-adaptive buffering capability .

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5:00pm **2D+MN+NS+SS-WeA9 Electrical and Structural Changes of Multilayer WSe_2 Transistors: Atmospheric Gas Adsorption and Long Term Aging**, ***Anna Hoffman****, M.G. Stanford, C. Zhng,* University of Tennessee Knoxville*; I. Ivanon,* Oak Ridge National Laboratory*; A.D. Oyedele, D.G. Mandrus,* University of Tennessee Knoxville*; L. Liang, B.G. Sumpter, K. Xiao,* Oak Ridge National Laboratory*; P.D. Rack,* University of Tennessee Knoxville

Interest in transition metal dichalcogenides (TMDs) for opto-electronic applications has been growing recently due to their unique properties and layered structure. Surface science and DFT simulations have corroborated p-type doping and n-type suppression of O_2 and H_2O adsorption in TMDs however, electrical characterization has not been fully investigated. This presentation will demonstrate the reversible suppression of n-type conduction in ambi-polar WSe_2 via water adsorption, which logically has a larger impact as the WSe_2 thickness decreases. Additionally, we observe a reversible and irreversible n-type suppression and p-type doping which we attribute to H_2O adsorption and isoelectronic oxygen chemisorption, respectively, at chalcogen vacancies during long term aging in atmosphere over 6 weeks. Finally, controlled oxygen plasma exposure is utilized to oxidize and p-type dope WSe_2. We will overview our device fabrication and electrical testing procedure, and transfer characteristics for our as-fabricated devices for various WSe_2 thicknesses in air and in vacuum will be illustrated. Long-term (6 week) electrical measurements in both air and vacuum are compared to the as-fabricated devices. Finally, complementary atomic force microscopy and Raman Spectroscopy are used to characterize the devices

5:20pm **2D+MN+NS+SS-WeA10 Ion Migration Studies in Exfoliated 2D Molybdenum Oxide via Ionic Liquid Gating for Neuromorphic Device Applications**, ***Cheng Zhang****, P.R. Pudasaini, A.D. Oyedele,* University of Tennessee Knoxville*; A.V. Ivelev, K. Xiao, T.Z. Ward,* Oak Ridge National Laboratory*; D.G. Mandrus,* University of Tennessee Knoxville*; O.S. Ovchinnikova,* Oak Ridge National Laboratory*; P.D. Rack,* University of Tennessee Knoxville

The formation of an electric double layer in ionic liquid (IL) can electrostatically induce charge carriers and/or intercalate ions in and out of the lattice which can trigger a large change of the electronic, optical and magnetic properties of materials and even modify the crystal structure. We present a systematic study of ionic liquid gating of exfoliated 2D molybdenum trioxide (MoO_3) devices and correlate the resultant electrical properties to the electrochemical doping via ion migration during the IL biasing process. A nearly nine orders of magnitude modulation of the MoO_3 conductivity is obtained for the two types of ionic liquids that are investigated. In addition, notably rapid on/off switching was realized through a lithium-containing ionic liquid whereas much slower modulation was induced via oxygen extraction/intercalation. Time-of-Flight Secondary Ion Mass Spectrometry confirms the Li intercalation. Results of short-pulse tests show the potential of these MoO_3 devices as neuromorphic computing elements due to their synaptic plasticity.

5:40pm **2D+MN+NS+SS-WeA11 Infrared Absorption of Nanometer-scale Thermally Reduced Graphene Oxide**, ***Erin Cleveland***, *J. Nolde, G. Jernigan, E. Aifer,* U.S. Naval Research Laboratory

Strong optical absorption is of fundamental importance to infrared (IR) sensors, and it has been well established that graphene is one of the strongest IR absorbing materials, with approximately 2.3% absorption in the IR and visible regions for a single layer. While reduced graphene oxide (RGO) may not have quite the same absorption strength as graphene on a layer-by layer basis, we believe that by controllably reducing the oxygen concentration within the GO films we can increase the absorption of the RGO film to approach that of graphene. RGO films, unlike graphene, however, can be made arbitrarily thick, allowing for much higher absorbance in a single pass. Here we explore the use of GO films of varying thickness and UHV annealing temperature to achieve near 100% midwave IR absorbance in a quarter-wave reflection filter structure consisting of an RGO film on top of a λ/4-thick SiO_2 layer deposited over a Ti/Pd mirror.

Graphene oxide (GO) is a two-dimensional network consisting of a graphene basal plane decorated with oxygen moieties in the forms of carbonyls, epoxies and hydroxyl groups resulting in variable number of $sp^2$and sp^3bonding geometries. Theory indicates that GO bandstructure and transport are strongly dependent on the ratio of the sp^2 and sp^3 bonding fractions, and therefore, by controllably removing specific oxygen groups, one can tune its electronic, optical, and chemical properties. While it is difficult to modify the oxygen concentration using wet chemical processing, e.g. using hydrazine, GO can be thermally reduced in H_2-N_2 forming gas with more precise control. However, this procedure, like chemical reduction promotes the occurrence of N and H impurities, as well as carbon vacancies within the graphene basal plane, significantly degrading the electronic quality of the film. Here, we use ultrahigh vacuum (<10^{-9} Torr) annealing to controllably reduce the oxygen concentration in GO films while introducing fewer defects. Not only does UHV annealing prevent the introduction of impurities, but after oxygen removal, dangling bonds tend to reform in hexagonal structure. UHV annealing also enables in-vacuo measurement by x-ray photoelectron spectroscopy (XPS) to precisely characterize the overall oxygen concentration and its distribution within alcohol, epoxy and carbonyl species. Following an 800°C UHV anneal for example, we find that the oxygen concentration is reduced to ~5%, and the layer spacing is equivalent to epitaxial graphene grown on the C-face of SiC.

6:00pm **2D+MN+NS+SS-WeA12 Dielectric Properties of Carbon Nanomembranes prepared from aromatic Self-Assembled Monolayers and their application in All-Carbon Capacitors**, ***Xianghui Zhang***, *P. Penner, E. Marschewski,* Bielefeld University, Germany*; T. Weimann, P. Hinze,* Physikalisch-Technische Bundesanstalt, Braunschweig, Germany*; A. Gölzhäuser,* Bielefeld University, Germany

Carbon nanomembranes (CNMs) are two-dimensional materials that are made by cross-linking self-assembled monolayers (SAMs) of aromatic molecules via low energy electron irradiation. Previous studies of the charge transport in molecular junction incorporating SAMs and CNMs of oligophenyl thiols has been carried out by using conical eutectic Gallium-Indium (EGaIn) top-electrodes[1] and conductive probe atomic force microscopy (CP-AFM)[2]. Additional investigations of the dielectric properties of pristine SAMs and CNMs were performed by impedance spectroscopy on EGaIn tunneling junctions. Here we demonstrate the fabrication and characterization of all-carbon capacitors (ACCs) composed of multilayer stacks of dielectric CNMs that are sandwiched between two types of carbon-based conducting electrodes: (1) trilayer graphene made by chemical vapor deposition and mechanical stacking; (2) pyrolyzed graphitic carbon (PGC) made by pyrolysis of cross-linked aromatic molecules. The junction area is defined by the width of electrode ribbons, ranging from 1 to 2500 μm^2, and the separation between two electrodes is tuned by the number of CNM layers. The frequency response of nanocapacitors was measured with an LCR meter. A dielectric constant of 3.5 and a capacitance density of up to 0.5 $\mu F/cm^2$ were derived from the junction capacitance. A dielectric strength of 6.2 MV/cm was determined. These results show the potential of carbon nanomembranes to be used as dielectric components in next-generation environment-friendly carbon-based molecular electronic devices.

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Electronic Materials and Photonics Division
Room 101A - Session EM+2D+SS-WeA

Wide and Ultra-Wide Bandgap Materials for Electronic Devices: Growth, Modeling and Properties

Moderators: Erica Douglas, Sandia National Laboratories, Rachael Myers-Ward, U.S. Naval Research Laboratory

2:40pm **EM+2D+SS-WeA2 2300 V Reverse Breakdown Voltage Ga_2O_3 Schottky Rectifiers**, ***Jiancheng Yang***[1], *F.R. Ren,* University of Florida*; M.J. Tadjer,* U.S. Naval Research Laboratory*; S.J. Pearton,* University of Florida*; A. Kuramata,* Tamura Corporation and Novel Crystal Technology, Inc., Japan

A reverse breakdown voltage of 2300 V with corresponding breakdown field of 1.15 MV/cm was demonstrated for 20 µm epi-β-Ga_2O_3 edge-terminated vertical Schottky rectifiers. This breakdown voltage is the highest ever reported for Ga_2O_3 rectifiers. Ga_2O_3 has an energy band gap of range 4.5 – 4.9 eV, which correlates to the theoretical breakdown electric field of ~8 MV/cm. The theoretical Baliga figure of merit (defined as V_B^2/R_{ON}, where V_B is the reverse breakdown voltage and R_{ON} is the on-state resistance) of Ga_2O_3 estimated to be 400% higher than GaN.[1] Previously reported, an unterminated Ga_2O_3 rectifier shown a breakdown voltage of 1600 V, and a field-plated Schottky diode has a breakdown voltage of 1076 V with the epi thickness 7 µm [2,3] This work has shown the improvement of the Ga_2O_3 vertical rectifiers breakdown voltage using a field-plate terminated approach with a lightly doped 20 µm Ga_2O_3 epitaxial layer . The edge-terminated Schottky rectifiers of various dimensions (circular geometry with diameter of 50-200 µm and square diodes with areas 4×10^{-3}- 10^{-2} cm^2) fabricated on 20µm lightly doped (n=2.10×10^{15} cm^{-3}) β-Ga_2O_3 epitaxial layers grown by hydride vapor phase epitaxy on conducting (n=3.6×10^{18} cm^{-3}) Ga_2O_3 substrates grown by edge-defined, film-fed growth. The R_{ON} for these devices was 0.25 Ω-cm^2, leading to a figure of merit (V_B^2/R_{ON}) of 21.2 MW/cm^2. The Schottky barrier height with the Ni/Au based metallization was 1.03 eV, with an ideality factor of 1.1 at room temperature. The Richardson's constant of 43.35 A/cm-K^2 was extracted from the temperature dependent forward IV. The breakdown voltages for the different size devices ranged from 1400-2300V, with a general, but not a linear trend of decreasing breakdown voltage for larger area rectifiers. The diode reverse recovery time of ~22 ns was measured by switching the diode from +2V to -2V.

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3:00pm **EM+2D+SS-WeA3 Characterization of β-$(Al,Ga,In)_2O_3$ Epitaxial Films for UV Photodetector Applications**, ***Luke Lyle***, *L.M. Porter, R. Davis,* Carnegie Mellon University*; S. Okur, G.S. Tompa,* Structured Materials Industries, Inc.*; M. Chandrashekhar, V. Chava, J. Letton,* University of South Carolina

β-Ga_2O_3 has garnered increased attention over the last few years due to its ultra-wide bandgap of ~5.0 eV and the ability to grow Ga_2O_3 single crystals from the melt. In addition to its desirability for high power electronics, Ga_2O_3 is well suited for solar-blind UV photodetectors. These detectors are coveted by numerous industries and the military for applications ranging from flame- and missile-plume detection to ozone hole monitoring. In this study we have grown $(Al,Ga,In)_2O_3$-based alloy epitaxial films on sapphire via metalorganic chemical vapor deposition (MOCVD) to investigate their potential application for wavelength-tunable UV photodetectors. The films were characterized structurally, optically, and chemically using x-ray diffraction (XRD), optical transmittance, and energy dispersive x-ray spectroscopy (EDX). Based on XRD and EDX results, β-$(Al_xGa_{1-x})_2O_3$, β-$(In_xGa_{1-x})_2O_3$, and β-Ga_2O_3 epitaxial films with compositions through x = 0.29 (for Al) and x = 0.13 (for In) were grown. The optical bandgap was found to correspondingly vary between 5.5±0.1 and 4.3±0.3 eV, as a function of composition. MSM- and Schottky-based solar-blind UV photodetectors were also fabricated on selected films. The devices showed responsivities up to 1E5 A/W and quantum efficiencies up to 6E5 at 220 nm from a deuterium lamp. The wavelength tunability of the photodetectors is currently being investigated and will be discussed in this presentation.

[1] **National Student Award Finalist**

3:20pm **EM+2D+SS-WeA4 High Three-terminal Breakdown Voltage Quasi-two-dimensional β -Ga_2O_3 Field-effect Transistors with a Dual Field Plate Structure**, ***Jinho Bae,*** Korea University, Republic of Korea*; H.W. Kim, I.H. Kang,* Korea Electrotechnology Research Institute (KERI), Republic of Korea*; G.S. Yang, S.Y. Oh, J.H. Kim,* Korea University, Republic of Korea

β-Ga_2O_3 is an intriguing material because of its large direct bandgap (4.85 eV), high breakdown field (~8 MV/cm) and excellent thermal and chemical stability. Baliga's figure of merit of β-Ga_2O_3 is 3214.1, superior to those of other materials such as GaN (846.0) or SiC (317.1). Although β-Ga_2O_3 is not a van der Waals material, β-Ga_2O_3 can be mechanically exfoliated from single crystal substrate into thin layer due to the large anisotropy of the unit cell. Quasi-2D β-Ga_2O_3 devices shows superior electrical properties and robustness in harsh environment, which shows potential of β-Ga_2O_3 as nanoscale power devices. However, quasi-2D β-Ga_2O_3 power devices show premature breakdown due to the electric field concentration. Adopting multiple field plates to relieve the electric field concentration and prevent premature breakdown greatly enhance the performance of power devices, which can be applied to β-Ga_2O_3 nanoelectronic power devices.

H-BN has been used as a dielectric material of 2D devices due to its excellent thermal conductivity and high dielectric constant, as well as atomically flat surface, which can be obtained through mechanical exfoliation. In our work, we used h-BN as a gate field plate dielectric layer by selective transfer on β-Ga_2O_3 channel using PDMS film. SiO_2 dielectric layer was deposited on devices followed by metal deposition for source field plate structure. By applying dual field plate structure, β-Ga_2O_3 devices can show excellent performance in high voltage condition.

β-Ga_2O_3 MESFETs with h-BN gate field plate were fabricated by using the β-Ga_2O_3 and h-BN flakes obtained from respective crystals. Ohmic metal was deposited on mechanically exfoliated β-Ga_2O_3 flakes, followed by precise positioning of exfoliated h-BN flakes on the channel. Gate field plate was fabricated with a part of the electrode overlapped with h-BN. Dual field plate structure was fabricated after deposition of SiO_2 and source field plate metal. Fabricated devices showed excellent output and transfer characteristics even after one month storage, which shows excellent air-stability. Three-terminal off-state breakdown voltage of fabricated device was measured, which shows improvement in breakdown voltage. The electric field distribution was calculated by Silvaco Atlas framework to study the effect of dual field plate on electric field, which explains the improvement of breakdown voltage in those structure. In this study, we present that the performance of β-Ga_2O_3 MESFET as a power device can be improved by adopting dual field plate structure, paving a way to the high-power nanoelectronic β-Ga_2O_3 devices. The details of our work will be discussed in the conference.

4:20pm **EM+2D+SS-WeA7 GaN Vertical Device Technology and its Future**, *S.C. Chowdhury,* ***Dong Ji,*** UC Davis **INVITED**

Vertical GaN devices are ideal for high power applications owing to their wide bandgap-originated material properties, similar to SiC. What makes GaN vertical devices more attractive than SiC, is the capability to offer bulk regions with electron mobility over 1200cm^2/V·sec. Due to higher carrier mobility made possible by superior growth techniques, the figure of merit offered by GaN diodes or FETs is higher compared to SiC counterparts. From TCAD drift diffusion simulation we have shown the advantage of GaN devices become rapidly significant over SiC diodes at higher voltages. In our experimental studies we have successfully demonstrated transistors blocking over 1.4kV.

In this presentation, we will go over various types of vertical devices for power conversion that we are pursuing in our group and go over the achievements and challenges in each.

CAVETs were the first vertical devices[1] that demonstrated the potential of GaN in these technology. CAVETs are realized with Mg-ion implanted [2] current blocking layers (CBLs) with regrown channel. Alternatively they can have Mg-doped CBLs with a regrown channel layer on a trench. In our trench CAVETs we have successfully blocked up to 880V with an R_{on} less than 2.7milli-ohm cm^2.

To date, most successful results in GaN vertical devices have come out of MOSFETs, which traditionally rely on inversion channels. MOSFETs with an un-doped GaN interlayer as a channel and in-situ MOCVD oxide, called OG-FET have demonstrated superior performance with low specific on-state resistance (R_{on}) Over 1.4kV blocking with an R_{on} less than 2.2milli-ohm cm^2 was recently demonstrated by our group where the role of channel mobility got highlighted[3].

One of common issue in all these devices is the realization of a robust buried p-n junction, which we will also go over along with other challenges faced by each of these device types and discuss paths to overcome those.

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5:00pm **EM+2D+SS-WeA9 Effects of Proton Irradiation Energy on SiN_x/AlGaN/GaN Metal-insulator-semiconductor High Electron Mobility Transistors**, ***Chaker Fares,*** *F.R. Ren,* University of Florida*; J.H. Kim,* Korea University, Republic of Korea*; S.J. Pearton,* University of Florida*; C.F. Lo, J.W. Johnson,* IQE*; G.S. Yang,* Korea University, Republic of Korea

The effects of proton irradiation energy ranging from 5 to 15 MeV on the electrical properties of SiNx/AlGaN/GaN metal-insulator-semiconductor high electron mobility transistors (MISHEMTs) using in-situ grown silicon nitride as the gate dielectric were studied. In applications such as satellite-based communication, remote sensing, radar technology, and nuclear energy production, microelectronics that are resistant to radiation must be utilized. Of the many materials and device architectures previously investigated, AlGaN/GaN high electron mobility transistors (HEMTs) show significant potential for environments where radiation hardness, elevated temperature, and high-power operation are required. Although several studies have been performed to analyze how HEMTs respond to irradiation damage, data on the effects of proton irradiation energy on MISHEMTs are scarce. In this study, AlGaN/GaN MISHEMT samples were irradiated at various proton irradiation energies at a fixed dose of 2.5×10^{14} cm^{-2} to determine the effects on device performance. After proton irradiation, all devices were functional and showed minimal degradation compared to previous reports of HEMTs irradiated at similar conditions.The dc saturation current was reduced by 10.4, 3.2 and 0.5% for MISHEMTs irradiated with proton energies of 5, 10, and 15 MeV, respectively. Device performance degradations were more pronounced in the irradiated samples under high-frequency operation. At a frequency of 100 KHz, the saturation drain current reduction at a gate voltage of 3 V was 40%, 19% and 17% after proton irradiation at 5, 10, and 15 MeV, respectively. At higher duty cycles, the drain current reduction is less severe. The results of this study demonstrated the device reliability of AlGaN/GaN MISHEMTs in environments where a resilience to radiation is required.

5:20pm **EM+2D+SS-WeA10 Cesium-Free III-Nitride Photocathodes Based on Control of Polarization Charge**, ***Douglas Bell,*** Jet Propulsion Laboratory, California Institute of Technology*; E. Rocco, F. Shahedipour-Sandvik,* SUNY Polytechnic Institute*; S. Nikzad,* Jet Propulsion Laboratory, California Institute of Technology

III-nitride photocathodes are well-suited for ultraviolet (UV) detection, with commercial, defense, and astronomical applications. Photocathodes detect light by absorbing photons which create electron-hole pairs, and emitting those electrons into vacuum, where they are detected and amplified by a gain-producing device such as a microchannel plate. This type of device is capable of ultra-low dark current and enables photon counting. The wide bandgaps available in the AlGaN family provide intrinsic solar blindness, and the long-wavelength cutoff may be tuned by control of composition.

Among other properties, negative electron affinity (NEA) is desirable for these structures in order to maximize quantum efficiency (QE), or the number of electrons emitted per incident photon. Normally surface cesiation is used to create low or negative electron affinity of the GaN photocathode surface; however, the resulting highly reactive surface must be protected from air during fabrication and use, necessitating a sealed-tube configuration. Even so, the reactive surfaces of these devices cause degraded performance over time. Cesium-free photocathodes would offer lower cost, smaller size and mass, improved robustness, and greater chemical stability, in addition to the major advantages of higher QE and longer lifetimes.

We will report on the use of polarization engineering in order to achieve high QE without the use of Cs. We will discuss progress in design, fabrication, and characterization of polarization-engineered III-nitride photocathodes. An important component of these designs is the use of N-polar GaN and AlGaN. The nitride polarity affects the interface and surface polarization charge, and the ability to achieve low electron affinity depends critically on control of this charge. Designs using polarization charge engineering also enable optimization of the near-surface potential to

further increase QE. We will describe the growth challenges of N-polar GaN and AlGaN and its implementation in photocathode devices. We will present results demonstrating high (>15%) QE for non-cesiated N-polar GaN photocathodes, with a clear path toward higher efficiency devices.

5:40pm **EM+2D+SS-WeA11 Current Enhancement for Ultra-Wide Bandgap AlGaN High Electron Mobility Transistors by Regrowth Contact Design**, ***Erica Douglas***, *B. Klein, S. Reza, A.A. Allerman, R.J. Kaplar, A.M. Armstrong, A.G. Baca,* Sandia National Laboratories

Recently, ultra-wide bandgap (UWBG) materials, such as Al-rich AlGaN with bandgaps approaching 6 eV, are being investigated to drive high-power electronic applications to even higher voltages, due to increased critical electric field compared to wide bandgap materials, such as GaN.[1] However, challenges have been encountered with Al-rich AlGaN, and in particular an increase in contact resistance as the bandgap for heterostructures increases.[2] High contact resistance ultimately limits the performance that can be achieved for these novel heterostructure-based devices, as source and drain resistances can be dominated by Ohmic contacts. While planar metal stacks with a rapid thermal anneal have shown some level of success, a complimentary approach using doped regrowth for the Ohmic contact regions with materials of lower bandgap has also shown a potential path for lowering contact resistance.[2] Our work explores regrown Ohmic contacts composed of lower bandgap Si-doped GaN to $Al_{0.85}Ga_{0.15}N/Al_{0.7}Ga_{0.3}N$ heterostructures , achieving a maximum saturated drain current of ~ 45mA/mm. Additionally, we demonstrate the ability to increase the saturated drain current almost 3X (from ~45 mA/mm to ~130 mA/mm) for UWBG HEMTs through a circular perforation design as well as a comb-type structure by means of regrowth contact design engineering.

[1] R. J. Kaplar, *et. al*, "Review—Ultra-Wide-Bandgap AlGaN Power Electronic Devices," ECS J. Solid State Sci. Technol., vol. 6, no. 2, pp. Q3061-Q3066, Jan. 2017.

[2] B. A. Klein, *et. al*, "Planar Ohmic Contacts to $Al_{0.45}Ga_{0.55}N/Al_{0.3}Ga_{0.7}N$ High Electron Mobility Transistors," ECS J. Solid State Sci. Technol., vol. 6, no. 11, pp. S3067-S3071, Aug. 2017.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

6:00pm **EM+2D+SS-WeA12 Understanding Homoepitaxial GaN Growth**, ***Jennifer Hite***, *T.J. Anderson, M.A. Mastro, L.E. Luna, J.C. Gallagher, J.A. Freitas,* U.S. Naval Research Laboratory*; C.R. Eddy, Jr.,* U. S. Naval Research Laboratory

The availability of high quality, free-standing GaN substrates opens windows for new device applications in III-nitrides, especially in vertical structures. With the introduction of these native substrates, the properties of nitrides are no longer dominated by defects introduced by heteroepitaxial growth. However, additional materials challenges are coming to the forefront that need to be understood and surmounted in order to allow homoepitaxial devices to achieve their full potential.

In order to enable device-quality epitaxial layers, a deeper understanding of substrate preparation and the effects of the substrate and growth initiation on the characteristics of the epitaxial layers is required for metal organic chemical vapor deposition (MOCVD) growth of homoepitaxial films. We investigate these effects on epi morphology, uniformity, and impurity incorporation at the interface and in the films. Although the initial substrate factors influencing the epi can be subtle, they can have far reaching impact on device performance. Additionally, the interface between substrate and epitaxy is examined to enable reduction of unintentional impurity incorporation, especially Si, at this surface. By studying these effects using wafers from several different vendors, with substrates from both hydride vapor phase epitaxy (HVPE) and ammonothermal techniques, an understanding of the requirements for device quality MOCVD homoepitaxy can be determined.

MEMS and NEMS Group
Room 202B - Session MN+2D+AN+NS-WeA
IoT Session: MEMS for IoT: Chemical and Biological Sensing

Moderators: Robert Davis, Brigham Young University, Sushma Kotru, The University of Alabama

2:20pm **MN+2D+AN+NS-WeA1 BioMEMS for Eye Applications**, ***Yu-Chong Tai***, California Institute of Technology **INVITED**

The field of Micro-Electro-Mechanical Systems (MEMS) has advanced tremendously for the last 20 years. Most noticeably, however, the field has mostly advanced in microsensors such as pressure sensors, accelerometers, gyros, microphones for cell phone and smart instrumentation applications. Looking forward though, in my opinion, one future direction of MEMS/NEMS is for micro biomedical devices. Among many possible biomedical applications, one challenging but promising branch is micro implants. Why micro implants? Body tissues (especially neurons), once severely damaged, do not repair or regenerate easily and often leave behind permanent debilitating deficits. Engineering implant technologies to interface intact tissues and/or to replace defective functions have continued to be the main solutions for many diseases. As our world is facing more severe aging population problems, significant growth in implant applications is foreseeable. As a matter of fact, there are already many existing commercially available implants such, as pacemakers and cochlear implants, but they all have a lot to improve. For examples, cardiovascular implants like defibrillator and pacemakers are still bulky, mechanically rigid, power hungry, and functionally limited. The future implants should be even smaller, flexible, power efficient and more versatile so that they can be used at places not possible before. This talk will review the research of implants done at the Caltech MEMS lab. More specifically, this talk will focus on bioMEMS implant devices to treat eye diseases. Examples of devices will cover the four major ophthalmic diseases, i.e., cataract, glaucoma, age-related macular disease and diabetic retinopathy that make of close to 80% of world blindness. It is believed that BioMEMS can also have many other opportunities for other organs in our body too.

3:00pm **MN+2D+AN+NS-WeA3 Real-Time, Single Cell, Size Measurements using a Facile, Multimode Microwave Resonator**, ***Selim Hanay***, *H. Aydogmus, A. Secme, H.S. Pisheh, M. Kelleci, U. Hatipoğlu,* Bilkent University, Turkey

In this study, a facile microwave sensor is designed and fabricated to detect transient cells one by one and extract their morphological and electrical properties in real time, without labeling. Multiple modes can be measured by multiplexing the electronic frequencies to obtain multiple analytic parameters at the same time. Our simple fabrication technique obviates the need to complex fabrication process.

A microwave sensor, in the form of a microstrip line resonator, is constructed by fixing copper tape at the back and the front side of a 1-mm thick glass slide. The backside is covered entirely with the tape to form a ground plane; on the front side, a copper tape was thinned within a few mm, extended across the slide and terminated with SMA feed through. On the front side, just below the copper tape, five capillary tubes are placed to transport the cells into the active sensing region. Microwave signals are transmitted through the two SMA ports at the end of the glass slide, perpendicular to the flow. The resonator is formed by electrically shorting the input/output ports. An initial characterization of the device is done by using spectrum analyzer so that its first and second order mode frequencies are obtained.

A digital phase-locked loops (PLL) measurement system with PI controller was constructed to track the resonance frequencies of the first two modes simultaneously in real-time. The PLL system tracks the two modes of the microstrip line resonator to sense the frequency shifts originating from the passage of the cells in the capillary.

As a proof of concept, initial PLL measurements were done with DI water. As water flows through the tube, frequency shifts around 100 kHz were observed in both modes. Later on, wildtype *Skbr3* breast cancer cells were flown through the same capillary. Frequency shifts in both modes were the responses of the resonator to the passage of the *Skbr3* cells beneath microstrip-line. The ratio between the first and second mode frequency shifts can be used determine the location of each cell by two-mode theory. The analyzed data indicates almost a constant slope, verifying the positional response of the sensors. Moreover, the size distribution of the cells is cumulated around a contour line for constant size as expected.

Earlier, we had detected single cells and distinguished different oncogenic cell lines using a PDMS based device. With this work, single-cell detection and sizing are accomplished with a device paradigm that does not require any lithography, metal deposition under vacuum or precise alignment of electrodes.

We acknowledge funding from European Research Council (ERC) Starting Grant (REM, 758769).

4:20pm **MN+2D+AN+NS-WeA7 Magnetic Microsystems for Communications**, ***Rob Candler***, University of California at Los Angeles **INVITED**

We are witnessing a rapid expansion of embedded devices (IoT) that have a variety of functions but a common requirement, to communicate with one another. These devices will be connected on a scale previously unseen, and they will therefore require an approach to efficiently generate and receive electromagnetic waves in a small form factor. One such approach is to rethink the way electrically small antennas operate, shifting from a current-based antenna to a voltage-controlled multiferroic antenna. Multiferroics are material systems with coupled magnetic and electrical properties, and they offer a new route for the miniaturization of magnetic field-coupled devices. Multiferroic systems allow for the conversion of magnetic flux to a voltage (and vice versa) without the need of a wire loop, avoiding inefficiencies due to Ohmic loss. *In particular, strain-coupled heterostructures* of magnetostrictive and piezoelectric materials have received much attention, as they can offer magneto-electric coupling many order of magnitudes higher than found in single-phase materials. A rapidly emerging research space in multiferroics is the development of miniature wireless devices, such as antennas and energy harvesters, taking advantage of the efficient flux-to-voltage conversion of multiferroics. In this talk, I will present work showing the impact of multiferroic coupling on the ferromagnetic resonance in GHz Bulk Acoustic Wave resonators, as well as investigations in frequency mixing from non-linear multiferroic affects. These results are all in support of our goal create a microscale multiferroic antenna that is orders of magnitude more efficient than its classical antenna counterpart.

Furthermore, continued miniaturization of existing and emerging components that use magnets (atomic clocks, quantum computing, magnetic memory) will increase their sensitivity to external magnetic fields as well as the crosstalk between components. To address this need, we are developing techniques for on-chip magnetic shielding using multiple layers of permalloy. We will present recent results showing microscale magnetic shields fabricated by electroplating multiple permalloy layers into molds, as well as milliscale shields that were conformally electroplated on 3D printed sheaths.

5:00pm **MN+2D+AN+NS-WeA9 MEMS-Based Resonant Sensors for IoT Applications**, ***Oliver Brand***, *M. Kim, P. Getz,* Georgia Institute of Technology **INVITED**

The presentation discusses resonant microsensors, in which the measurand affects a characteristic of the resonance behavior of a resonant microstructure or a resonant circuit, such as its resonance frequency or quality factor. Resonant sensing is a very versatile sensing approach and can be adapted to a large variety of physical, chemical and biological measurands. Especially when using the resonance frequency as the sensing signal, high resolution is achievable since frequencies can be measured accurately. The presentation will highlight two possible implementations of resonant chemical sensors for Internet of Things (IoT) applications, a cantilever-based electromechanical resonator and a purely electrical L-C resonance circuit.

The first example is an electro-mechanical resonant chemical sensor based on a silicon hammerhead structure coated with a polymeric sensing film for the detection of volatile organic compounds. The presentation will highlight how proper selection of the resonance mode, in this case an in-plane vibration mode, and device geometry can improve device performance and how fast temperature modulations of the resonant sensors enable the observation of signal transients that contain additional analyte information. The sensors are fabricated using a CMOS-compatible bulk-micromachining process, have resonance frequencies between 400-800kHz and achieve sub-ppm limits of detection for select analytes.

The second example is a purely electrical resonant chemical sensor in form of a flexible and stretchable L-C (inductor-capacitor) sensor, which is battery free and can be wirelessly interrogated. To achieve stretchable sensor characteristics, the spiral inductor and interdigitated capacitor structures are formed by a liquid metal, eutectic gallium-indium (EGaIn). A subtractive reverse stamping technique is used to form the conducting liquid metal lines with dimensions as small as 2µm inside PDMS microchannels and a 3D heterogeneous integration technique is applied to vertically stack and electrically interconnect the capacitor and inductor structure. Liquid and gaseous analytes change the capacitance and are detected by wirelessly measuring the resonance frequency of the L-C circuit around 143MHz.

5:40pm **MN+2D+AN+NS-WeA11 Etched Silicon Microcolumn For Tunable Thermal Gradient Gas Chromatography**, ***Aaron Davis***, *P. Schnepf, P.S. Ng, R.R. Vanfleet, R.C. Davis, B.D. Jensen,* Brigham Young University

The connection of the digital and physical world will be strengthened by chemical sensors that can measure complex mixtures of molecules. Gas chromatography is the gold standard for identification of volatiles and gases. Conventional gas chromatography systems have unparalleled resolution, but are large and power intensive. Microcolumn gas chromatographs are more portable but have dramatically reduced resolution. Combining the resolution of conventional systems with the size factor of micro systems is important for improving the affordability and portability of high performance gas analysis. Recent work has demonstrated feasibility of high resolution separation of gases in a benchtop-scale short-column system by controlling thermal gradients through the column. In order to further decrease the size of a gas chromatography system, microfabrication techniques were used to demonstrate the fabrication of a thermally controllable micro-scale gas chromatographic column with a small footprint (3 cm square). To fabricate microcolumns we are using deep-reactive-ion-etching, nickel evaporation, and wafer bonding. The design of the 20 cm column utilizes 21 individually controllable thin film heaters and solid conduction cooling to produce the desired thermal profile.

2D Materials Focus Topic
Room 201B - Session 2D+EM+MI+MN+NS+SS-ThM
Novel 2D Materials

Moderator: Han Wang, University of Southern California

8:20am **2D+EM+MI+MN+NS+SS-ThM2 Controlled Growth of 2D Ni-Silicate and Silica Films on Ni_xPd_{1-x} (111) Substrates**, ***Chao Zhou***, *X. Liang, G.S. Hutchings, Z. Fishman, J.-H. Jhang, S. Hu, S. Ismail-Beigi, U.D. Schwarz, E.I. Altman,* Yale University

The discrete lattice constants and distinct chemical properties of different transition metal substrates hamper the systematic study of how the substrates can influence two-dimensional (2D) materials growth. The recent report of single-crystal epitaxial Ni-Pd alloy films with continuously tunable lattice constants open the possibilities to tackle this issue. Two-dimensional silica and transition-metal-doped silicate films prepared on metal substrates can be 2D analogues of porous bulk zeolites. In this research, 2D silica and Ni-silicate films were prepared on Ni_xPd_{1-x} (111) substrates under different growth conditions. After annealing in 2×10^{-6} Torr oxygen, Ni from the alloy substrates incorporates into the silica structure to form a crystalline 2D Ni-silicate structure, while an amorphous 2D silica bilayer can be observed after being annealed in 4×10^{-8} Torr oxygen. Density functional theory (DFT) was employed to model various silica and silicate phases on Ni_xPd_{1-x} (111) substrates. The results show that the 2D Ni-silicate films are thermodynamically stable on the substrates when the oxygen chemical potential is in the oxygen-rich range. In oxygen-deficient environments, 2D silica tends to form a stable Ni-free phase. With continuous control over the composition of NiPd alloy films, the surface strain applied on the Ni-silicate films through the lattice mismatch between the substrate and overlayer could also be continuously tuned. Only single-domain commensurate crystalline 2D Ni-silicate can be observed in zero or low-strain systems, while a second incommensurate crystalline domain which is rotated by 30° with respect to the commensurate domain can be observed when the lattice mismatch is over 1.85%.

8:40am **2D+EM+MI+MN+NS+SS-ThM3 Topological Materials**, ***Hsin Lin***, Institute of Physics, Academia Sinica **INVITED**

Topological materials host various novel quantum phases of electrons which are characterized by band topology and topologically protected surface/edge states. Despite recent progress, intense world-wide research activity in search of new classes of topological materials is continuing unabated. This interest is driven by the need for materials with greater structural flexibility and tunability to enable viable applications in spintronics and quantum computing. We have used first-principles band theory computations to successfully predict many new classes of topologically interesting materials, including Bi_2Se_3 series, the ternary half-Heusler compounds, $TlBiSe_2$ family, Li_2AgSb-class, and $GeBi_2Te_4$ family as well as topological crystalline insulator (TCI) SnTe family and Weyl semimetals TaAs, $SrSi_2$, $(Mo,W)Te_2$, Ta_3S_2, and LaAlGe family. I will also highlight our recent work on unconventional chiral fermions in RhSi and several material candidates for new TCI.

9:20am **2D+EM+MI+MN+NS+SS-ThM5 Few-Layer Rhenium Disulfide Synthesized Via Chemical Vapor Deposition**, ***Michael Valentin***, Army Research Laboratory; *A. Guan, A.E. Nguyen, I. Lu, C.S. Merida, M.J. Gomez,* University of California, Riverside; *R.A. Burke, M. Dubey,* Army Research Laboratory; *L. Bartels,* University of California, Riverside

Transition metal dichalcogenides (TMDs) are exciting new materials that have received much attention due to their semiconducting properties in the direct bandgap. Well-studied TMDs, such as molybdenum disulfide (MoS_2) and tungsten diselenide (WSe_2), exhibit a direct bandgap in the monolayer form, but an indirect bandgap in the bulk form. Rhenium disulfide (ReS_2), on the other hand, is a new TMD that is unique in its ability to retain a direct bandgap independent of thickness. By using chemical vapor deposition (CVD), few-layer ReS_2 is synthesized and characterized by optical methods such as Raman spectroscopy and photoluminescence. We also show characterization results for atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS), scanning electron microscope (SEM), transmission electron microscope (TEM), and electrical transport to determine thickness, crystallinity, homogeneity, and electrical characteristics for use in future flexible electronics.

9:40am **2D+EM+MI+MN+NS+SS-ThM6 Dipolar Disorder of a van-der-Waals Surface Revealed by Direct Atomic Imaging**, *M.A. Susner,* Air Force Research Laboratory; *M.A. McGuire,* ***Petro Maksymovych***, Oak Ridge National Laboratory

Recently, the family of transition metal thiophosphates –exhibiting ferroelecric, antiferromagnetic and correlated electron ground states – have gained attention as possible control dielectrics for the rapidly growing family of 2D and quasi-2D electronic materials [1]. Being van-der-Waals crystals, the surfaces of these materials can be created without dangling bonds, unlike those of complex oxides. Yet, because of robust insulating properties, the structure of their surfaces, the role of disorder, the structure of the topological defects in the order parameter and many other properties directly relevant to their prospective interfaces is almost entirely unknown.

Here we present the first atomically resolved imaging of $CuScP_2S_6$ s carried out using cryogenic non-contact atomic force microscopy. The surface exhibits good crystalline ordering at the atomic scale, revealing contrast on sub-unit cell level. The most remarkable property is long-range commensurate modulation of the surface morphology, with a topographic amplitude of only 2-3 pm. Combined with XRD analysis of the bulk and Monte-Carlo simulation of the Ising model on triangular lattice, we propose that the modulation arises from antiferroelectric polarization domains, albeit with frustrated long-range order. The key structural ingredient for this state is centrosymmetric position of Sc^{3+} within the layer, which forces the surrounding displacing Cu+1 ions to adopt a frustrated antiferroelectric state - in direct analogy frustrated magnetic systems. We will further discuss the peculiarities of nc-AFM imaging of this materials from the statistical analysis of the variation of images between scan, as well as the force-distance curve arrays. The possibility to directly visualize polar order opens broad opportunities to understand the atomistic aspect of ferroelectric, glassy and incommensurate phases in this material class, beginning with $CuInP_2S_6$ – which exhibits Curie temperature ~315K and giant negative electrostriction [2]. Research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy. Microscopy experiments were conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

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11:00am **2D+EM+MI+MN+NS+SS-ThM10 Advanced ARPES Analyzer and Momentum Microscope KREIOS 150 – Concepts and first results on layered materials and topological insulators**, ***Paul Dietrich***, *M. Wietstruk, T.U. Kampen, A. Thissen,* SPECS Surface Nano Analysis GmbH, Germany

Modern ARPES analyzers provide a high degree of parallelization in data acquisition, recording hundreds of energy and angle channels simultaneously. Additionally, integrated deflectors enable users to perform angle scanning perpendicular to the analyzer's entrance slit to record (k_x, k_y, E) data sets without sample rotation. However, the design of conventional analyzers implies a limited acceptance angle and corresponding accessible momentum space volume. Due to the trade-off between acceptance angle and angle resolution multiple changes in sample position and lens modes are necessary during a typical high resolution ARPES experiment. The new KREIOS 150 Energy Analyzer uses an extractor zoom lens design to overcome these limitations.

This new lens provides a full solid acceptance angle with highest angular resolution. In contrast to standard ARPES measurements with conventional hemispherical analyzers, electronic structure data from and beyond the 1st Brillouin zone is recorded without any sample movement. In addition the lens of such an instrument can work in a lateral imaging mode for microscopy as well. This enables navigation on the sample and reduces the size of the area under investigation in ARPES down to a few micrometers in diameter. This combination of large acceptance angle, high angular resolution and small acceptance area, makes this instrument the ideal tool for electronic structure studies on small samples or sample areas. The design is compact with a straight optical axis.

The capabilities of this instrument were tested at the UE 56/2 at the Bessy II synchrotron in Berlin. Specification tests show excellent angle and lateral resolution as well as small spot capability down to 2µm FOV. Subsequently

real live samples like Graphene on Germanium were measured. Even on macroscopically rough surfaces like Graphene on $NbSe_2$ excellent ARPES and X-PEEM results could be obtained. By taking advantage of the small spot capability of the KREIOS 150 meaningful band structure data has been recorded on such patchy samples.

Acknowledgements: We thank Yu. Dedkov (University of Shanghai, China) and M. Fonin (University Konstanz) for providing beamtime and samples for the measurements with KREIOS 150 at BESSY II.

11:20am **2D+EM+MI+MN+NS+SS-ThM11 Carbon Nanomembranes with Sub-nanometer Channels: 2D Materials for Water Purification with High Selectivity and Highest Permeance**, *Y. Yang, P. Dementyev, N. Biere, D. Emmrich, P. Stohmann, R. Korzetz, X.H. Zhang, A. Beyer, S. Koch, D. Anselmetti,* ***Armin Gölzhäuser,*** Bielefeld University, Germany

Clean water is a global challenge, and membrane filtration is a key technology to achieve it. Here, we report on carbon nanomembranes (CNMs) with sub-nanometer channels that prove to be excellent water filters, combining a high selectivity with an exceptionally high water permeance. The CNMs are fabricated via the cross-linking of terphenyl self-assembled monolayers [1], resulting in a ~1.2 nm thick membrane perforated by channels with diameters below ~0.7 nm and areal densities of $\sim 10^{18} m^{-2}$. When tested as filter membranes, it was found that the CNMs efficiently block the passage of most gases and liquids [2]. However, water passes through, and it does this with a record-breaking permeance of $\sim 1.1 \times 10^{-4}$ mol·m^{-2}·s^{-1}·Pa^{-1}. This suggests that water molecules translocate fast and cooperatively through the sub-nanometer channels.Assuming all channels in a TPT-CNMs are active in mass transport, we find a single-channel permeation of ~66 water molecules·s^{-1}·Pa^{-1}.We compare this with molecular transport through other carbon nanoconduits, such as carbon nanotubes or membrane proteins (aquaporins). As the fabrication of CNMs is scalable, their utilization opens a path towards the application of 2D-materials in energy-efficient water purification.

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11:40am **2D+EM+MI+MN+NS+SS-ThM12 Discovery of Dirac Monolayers and Elucidation of Functonalites by Advanced Soft X-ray Spectroscopy**, ***Iwao Matsuda,*** University of Tokyo, Japan **INVITED**

Vapor deposition of three-dimensional (3-D) crystal on a substrate often results in formation of the novel 2-D materials with intriguing electronic states. The approach has been well-known in the field of "Surface Science", which has attracted our attentions over the past decades. Triggered by fabrication of the graphene layers, researches on such monatomic sheets have extended to various kinds such as silicene, germanene and so on. Soft X-ray spectroscopies, such as photoemission spectroscopy, have been used to directly probe electronic states of monatomic layers and also to examine carrier dynamics under the *operando* condition. We recently observed Dirac Fermions in a 2-D boron sheet, borophene, that forms spontaneously on the Ag(111) surface. Furthermore, we found pairing of the Dirac cones due to Moire-periodic perturbations of the overlayer-substrate interactions. In the Cu_2Si monolayer, we also discovered the 2-D Dirac nodal line fermions that are protected by the mirror reflection symmetry. In the presentation. I will describe details of our research on the novel 2-D Dirac materials and introduce the advanced soft X-ray techniques that reveal their functionalities for developing devices.

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Magnetic Interfaces and Nanostructures Division
Room 203A - Session MI+2D-ThM

Magnetism at the Nanoscale

Moderator: Hendrik Ohldag, SLAC National Accelerator Laboratory

8:20am **MI+2D-ThM2 Magnetic Competition in $La_{0.7}Sr_{0.3}MnO_3$ Thin Films**, ***Mikel B. Holcomb,*** West Virginia University

$La_{0.7}Sr_{0.3}MnO_3$ is a strongly correlated ferromagnetic system, commonly proposed for many magnetoresistance applications. Utilizing many techniques (bulk magnetometry, neutron reflectometry and resonant x-ray magnetic scattering), we observe magnetic competition between different magnetic phases in many samples under various growth conditions. This competition results in inverted hysteresis loops (common in superparamagnetic nanoparticles) and negative remanent magnetization. While transmission electron microscopy images show pristine epitaxial growth, the data supports that there are regions of different magnetic order. This results in interesting magnetic measurements, that share similarities with ferrimagnets with competing magnetic lattices. Sample growth and optimization were supported by NSF (DMR-1608656), national facility measurements and theory were supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0016176, and optical measurements by American Chemical Society (PRF #56642-ND10). **We acknowledge the support of the National Institute of Standards and Technology, U.S. Department of Commerce, in providing the neutron research facilities used in this work.**

8:40am **MI+2D-ThM3 Ferromagnetism in 2D Materials**, ***Jiabao Yi,*** The University of New South Wales, Australia **INVITED**

Discovery of graphene has attracted wide interest of research in the family of 2D layered materials including TMDC (transition metal dichalcogenide), silicene, metal oxide and boron nitride. 2D materials have shown many extraordinary properties, such as high carrier mobility, extra-large mechanical strength and high thermal conductivity and excellent performance in energy storages. Due to its two-dimension nature and high carrier mobility, 2D materials are also very promising for spintronics devices. Graphene has shown long spin diffusion length and high spin injection efficiency [1]. Therefore, introducing magnetism into 2D materials becomes one of the research interests in 2D materials. Doping magnetic element into 2D materials is one of the effective methods to achieve magnetism. Most of the research focuses on theoretical calculations. In this presentation, I will introduce both theoretical calculations and experimental results on magnetic element doped 2D materials. From first principles calculations, it shows defects or defect complexes play important role in the magnetism [2]. In addition, ferromagnetism can be tuned by strain [3]. Experimentally, we observe room temperature ferromagnetism in magnetic element doped 2D materials. Especially, giant coercivity and extremely high magnetization have been observed in magnetic element doped MoS_2. Defects and shape anisotropy play critical roles in the high magnetization and coercivity [4,5].

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9:20am **MI+2D-ThM5 New Insights into Nanomagnetism by Low-temperature Spin-polarized Scanning Tunneling Microscopy**, ***Dirk Sander,*** Max Planck Institute of Microstructure Physics, Germany **INVITED**

Spin-polarized scanning tunneling microscopy at low temperature (8 K) and in high magnetic fields (6 T) is a powerful technique to investigate magnetic properties of individual nanoscale objects ranging in size form single atoms to several thousand atoms [1]. I focus on the magnetization reversal [2] and the spin-dependent electronic properties of bilayer Co [3], Fe-decorated Co and Fe islands on Cu(111). We find a novel noncollinear, helical magnetic order in the Fe islands, which is identified by a magnetic stripe contrast with a period of 1.28 nm [4,5] in bilayer islands. The periodicity increases to 2.2 nm in three-layer thick Fe islands [6]. The high spatial resolution of the spin-polarized scanning tunneling spectroscopy in combination with theory reveals the significance of structural and electronic relaxation [7] for the magnetic anisotropy, for subtle balances between ferromagnetic and antiferromagnetic exchange interaction, and for spin-dependent transport properties [8] of individual, single nanostructures.

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11:00am **MI+2D-ThM10 Materials Optimization to Form Skyrmion and Skyrmion Lattices***, **Eric Fullerton,*** University of California at San Diego **INVITED**

There is increasing interest in materials systems where magnetic skyrmions can be observed. I will discuss two materials systems where we observe chiral spin structures at room temperature. The first system is ferrimagnetic Fe/Gd-based multilayers where we observe sub-100-nm skyrmions and skyrmion lattices. However, the chirality of the skyrmions are random indicating they are dipole stabilized (similar to of bubble memory in the 1970's) as opposed to by DMI that favors a fixed chirality. This further allows the formation of bi-skyrmions which result from the merging of two skyrmions of opposite chirality and anti-skyrmions. We find that there is a transition from stripe domains to a skyrmion lattice and then individual skyrmions with magnetic fields and this behavior is sensitive to alloy composition, film thickness, temperature, and field history and only emerges in a narrow range of parameters. Using micromagnetic modeling we are able to quantitatively reproduce our experimental observations. The modeling suggests that the domain wall is Bloch-like in the center of the films but broadens and transitions to more Néel-like towards the surface forming closure domains. The Bloch-like centers have an equal population of the two helicities while the Néel-like part of the walls will have the same helicity at the top of the film and the opposite helicity at the bottom of the film which allows coupling to spin-orbit-torque layers. The second system is Pt/Co(1.1 nm)/Os(0.2 nm)/Pt heterostructures. Using Kerr microscopy to observe skyrmions for a narrow temperature and field range. With relatively low currents, it is possible to generate and move these skyrmions both within patterned wires and full films and we further have observations of the skyrmion Hall effect. The research is done in collaboration with S. A. Montoya, R. Tolley, J. Brock, S. Couture, J. J. Chess, J. C. T Lee, N. Kent, D. Henze, M.-Y. Im, S.D. Kevan, P. Fischer, B. J. McMorran, V. Lomakin, and S. Roy and is supported by the DOE.

11:40am **MI+2D-ThM12 Giant Magnetostriction and Low Loss in FeGa/NiFe Nanolaminates for Strain-Mediated Multiferroic Micro-Antenna Applications***, **Kevin Fitzell*** [1]*, C.R. Rementer,* University of California, Los Angeles*; N. Virushabadoss,* University of Texas at Dallas*; M.E. Jamer,* National Institute of Standards and Technology (NIST)*; A. Barra,* University of California, Los Angeles*; J.A. Borchers, B.J. Kirby,* National Institute of Standards and Technology (NIST)*; G.P. Carman,* University of California, Los Angeles*; R.M. Henderson,* University of Texas at Dallas*; J.P. Chang,* University of California, Los Angeles

The ability to reduce the size of antennae would enable a revolution in wearable and implantable electronic devices. Multiferroic antennae, composed of individual ferromagnetic and piezoelectric phases, could reduce antenna size by up to five orders of magnitude through the efficient coupling of magnetization and electric polarization via strain. This strategy requires a low-loss magnetic material with strong magnetoelastic coupling at high frequency.

Galfenol ($Fe_{84}Ga_{16}$ or FeGa) is a promising candidate material due to its large magnetostriction (>200 ppm), large piezomagnetic coefficient (>3 ppm/Oe), and high stiffness (>50 GPa), but it is highly lossy in the GHz regime. On the other hand, Permalloy ($Ni_{81}Fe_{19}$ or NiFe) is a soft magnetic material that has very low loss in the GHz regime (ferromagnetic resonance linewidth <20 Oe) but almost no magnetostriction. In this work, nanoscale laminates containing alternating layers of FeGa and NiFe were fabricated via DC magnetron sputtering to combine the complementary properties of the two magnetic phases. Optimized magnetic laminates were shown to exhibit a small coercive field (<20 Oe), narrow ferromagnetic resonance linewidth (<40 Oe), and high relative permeability (>400) (Rementer et al., 2017). In addition, optical magnetoelastic measurements of these laminates confirmed the presence of strong magnetostriction; relative to single-phase FeGa, these laminates represent a threefold enhancement in magnetostriction at saturation and up to a tenfold enhancement at low magnetic fields.

Multiferroic composites incorporating these magnetic laminates were then studied via polarized neutron reflectometry, demonstrating coherent rotation of the individual layers' magnetization with an applied electric field across distances much larger than the exchange length of either material. Micromagnetic and finite element simulations support the experimental results, showing coherent rotation of the magnetization with only small deviations with thicker NiFe layers. Subsequent integration of these laminates into strain-mediated multiferroic antennae confirmed the absorption of electromagnetic and acoustic waves, showing great promise for the use of FeGa/NiFe laminates in micro-scale communications systems.

12:00pm **MI+2D-ThM13 Structural and Electronic Origin of Stable Perpendicular Magnetic Anisotropy in Pt/Co/Pt magnetic ultra-thin film with Ti Buffer Layer***, **Baha Sakar,*** Gebze Technical University, Turkey*; Z. Balogh-Michels, A. Neels,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland*; O. Öztürk,* Gebze Technical University, Turkey

In this work, Pt and Co based multilayer samples with perpendicular magnetic anisotropy (PMA) are prepared. The aim of the work is the optimization and stabilization of the magnetic properties. Highly stable and repeatable PMA samples are demanded for standardization and calibration of magnetic measurements. For this purpose, Pt/Co/Pt (pcp) and Ti/Pt/Co/Pt (tpcp) samples are prepared on naturally oxidized Si(111) substrates by using magnetron sputtering. Electronic structures and elemental composition of the sample surfaces are investigated by X-Ray Photoelectron Spectroscopy. The same technique is also used for thickness calibrations of depositions. Magnetic properties of the samples are investigated by using Magneto-Optical Kerr Effect method. Orientations of the grains are important for defining the magnetic easy axis of a magnetic material. Typical symmetric XRD scans are not suitable for very thin films (<10 nm) since the signal to background ratio is low. For this reason, structural properties of the films are analyzed by using grazing angle XRD and in-plane XRD reciprocal space mapping.

Samples with the titanium buffer layer (tpcp) have perpendicular magnetic anisotropy where the pcp samples have in-plane magnetization. Structural differences in the presence of Ti layer are the strong preferred orientation for Pt, while the pcp film is random oriented. Multiple Co reflections are also visible for the pcp film. These confirmed a 111 fiber texture for the Pt in case of the tpcp sample. Contrary to that multiple Pt rings are observed for the pcp sample, which agrees with a random oriented nanocrystalline film. The lack of a texture explains the magnetic behavior.

Samples prepared in this work are used/using and studied within a joint research project, EMPIR SIB05 NanoMag funded by EURAMET.

MEMS and NEMS Group
Room 202B - Session MN+2D+AN+MP+NS-ThM
Optomechanics and 2D NEMS

Moderator: Max Zenghui Wang, University of Electronic Science and Technology of China

8:00am **MN+2D+AN+MP+NS-ThM1 Towards Microwave to Telecom Wavelength Quantum Information Transfer using Cavity Optomechanics***, **John Davis,*** University of Alberta, Canada **INVITED**

The past few years have seen the rapid maturation of quantum information processors, particularly in the category of superconducting microwave circuits. With claims from leading companies that they will commercialize quantum processors in the next five years, we must wonder what quantum technologies should be developed in tandem to fully utilize these processors. For example, we are all acutely aware that while our personal computers are powerful, they are considerably more useful and interesting when networked together. So how can we likewise network quantum processors? Especially since the microwave signals of superconducting processors cannot be transmitted at room temperature without thermal decoherence. What if instead, one could link superconducting processors together through existing fiber-optic networks, which are already capable of long distance quantum information transfer? Hence the development of a transducer of quantum information from the microwave to telecom domain has become highly desirable. I will describe the current state of microwave to optical transducers, and how our lab is working towards this

[1] **Falicov Student Award Finalist**

goal. Specifically, I will discuss the progress and challenges associated with the development of fiber-coupled telecom-wavelength cavity optomechanical resonators, and 3D superconducting microwave cavities, operating at millikelvin temperatures. I will also discuss ongoing collaborations that could enable implementation of quantum information transducers in a large-scale fiber network in Alberta.

11:20am **MN+2D+AN+MP+NS-ThM11 Reconfigurable Resonant Responses in Atomic Layer 2D Nanoelectromechanical Systems (NEMS)***, **Zenghui Wang**,* University of Electronic Science and Technology of China*; R. Yang, P.X.-L. Feng,* Case Western Reserve University

Atomic layer semiconducting crystals have emerged as a new class of two-dimensional (2D) materials, exhibiting great promises for both fundamental research and technological applications. Their outstanding electromechanical properties make these materials ideal for constructing novel 2D NEMS, providing opportunities for leveraging their unique device properties across multiple information-transduction domains, at scales down to individual atomic layers. One particularly interesting category of 2D NEMS is 2D nanoelectromechanical resonators, which hold potentials for making the next generation RF signal transduction and processing components, with miniaturized size, ultra-low power consumption, and compatibility with transparent and flexible circuits.

Towards future applications in the 5G era, multi-band RF signal handling capability is desired, as the number of bands each mobile device need to have access to significantly increases, and it would be impractical to simply increase the number of RF components that can only function under one RF frequency, as the space required for mounting such components scales with the number of bands. Therefore, ultralow-power tunable and reconfigurable RF devices that can adapt to different frequencies would be one solution to this challenge.

Here we present experimental demonstration of nanomechanical resonators based on layered MoS_2 atomic crystals that have reconfigurable resonant responses. By carefully studying the temperature-dependent frequency response in such MoS_2 resonators[1], we discover clear, repeatable hysteretic behavior as the device temperature is changed[2]. Leveraging this phenomenon, we achieve switchable resonance frequency f_{res} in such devices by using heating and cooling pulses. Specifically, for an example MoS_2 resonator, during heating pulses, the f_{res} decreases to ~20MHz. Once the device recovers to room temperature, f_{res} stabilizes at ~26MHz. During cooling pulses, f_{res} increases to ~29MHz, and upon reverting to room temperature f_{res} stays at ~24.5MHz, which is clearly different than the other room temperature state. Our findings suggest that such atomic-layer MoS_2 NEMS resonators could be used towards developing reconfigurable RF components whose frequency response can be switched between different states.

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11:40am **MN+2D+AN+MP+NS-ThM12 Cavity Optomechanics: Dynamics and Applications***, **Eyal Buks,*** Israel Institute of Technology, Israel **INVITED**

The field of cavity optomechanics deals with a family of systems, each composed of two coupled elements. The first one is a mechanical resonator, commonly having a low damping rate, and the second one is an electromagnetic cavity, which typically is externally driven. Both radiation pressure and bolometric force can give rise to the coupling between the mechanical resonator and the cavity. In recent years a variety of cavity optomechanical systems have been constructed and studied, and phenomena such as mode cooling, self-excited oscillation, and optically induced transparency have been investigated. The first part of the talk will be devoted to some dynamical effects including synchronization and intermittency. In the second part some applications of optomechanical cavities for sensitive sensing will be discussed.

2D Materials Focus Topic
Room 201B - Session 2D+EM+MN+NS-ThA
Novel Quantum Phenomena in 2D Materials

Moderator: Hsin Lin, Institute of Physics, Academia Sinica

2:20pm **2D+EM+MN+NS-ThA1 Double Indirect Interlayer Exciton in a $MoSe_2/WSe_2$ van der Waals Heterostructure**, ***Aubrey Hanbicki***, *H.-J. Chuang, M. Rosenberger, C.S. Hellberg, S.V. Sivaram, K.M. McCreary, I. Mazin, B.T. Jonker,* Naval Research Laboratory

Tailoring semiconductor heterostructures for specific functionalities has led to varied opto-electronic devices including solar cells, photodetectors, light-emitting diodes and lasers. An emerging class of heterostructures involves monolayer semiconductors such as many of the transition metal dichalcogenides (TMDs) which can be combined to form van der Waals heterostructures (vdWHs). vdWHs offer novel functionalities making them promising hosts for future devices. One unique new heterostructure property is an interlayer exciton (ILE), a spatially indirect, bound electron-hole pair with the electron in one TMD layer and the hole in the other. Here, using state-of-the-art preparation techniques, we are able to resolve emission from the ILE in a $MoSe_2/WSe_2$ heterostructure into two distinct peaks separated by 24 meV at zero field. These peaks have nearly equal intensity, indicating they are of common character, and have *opposite* circular polarizations when excited with circularly polarized light. *Ab initio* calculations successfully account for these observations – they show that both emission features originate from excitonic transitions that are indirect in momentum space and are split by spin-orbit coupling. Also, the electron is strongly hybridized between both the $MoSe_2$ and WSe_2 layers, with significant weight in both layers, contrary to the commonly assumed model. Thus, the transitions are not purely interlayer in character. This work represents a significant advance in our understanding of the static and dynamic properties of TMD heterostructures.

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

2:40pm **2D+EM+MN+NS-ThA2 Comparison of A- and B-exciton Intensity and Polarization in Transition Metal Dichalcogenide Monolayers and Heterostructures**, ***Kathleen McCreary***, *A.T. Hanbicki, S.V. Sivaram, B.T. Jonker,* U.S. Naval Research Laboratory

We survey a large number of monolayer TMDs to better understand the conditions responsible for various emission characteristics that have been reported in literature. We find that the intensities for both A- and B- peak emission vary widely as a result of sample-to-sample variations. However, a measurable B-peak intensity is evident in all samples. There is a clear linear relationship between the two peak intensities. The emission from the dominant A-peak is commonly several orders of magnitude higher than B-peak emission, resulting in B/A-intensity ratios well below 1%. Yet, as the A-peak intensity decreases, the ratio of B/A monotonically increases, and we observe a B/A ratio up to 30% in monolayer MoS_2. The A-excitonic emission is further quenched when $MoS_2$is incorporated into an $MoS_2/MoSe_2$heterostructure, where we observe comparable A- and B-peak intensities. We attribute these variations to differences in exciton recombination times, clarifying contradictory reports regarding the accessibility and significance of B-peak emission. Furthermore, we observe a high degree of valley polarization in both B-exciton emission in isolated monolayers and A-exciton emission in heterostructures, consistent with our model detailing the rapid exciton lifetimes in B-emission and van der Waals heterostructures.

Supported by core programs at NRL and the NRL Nanoscience Institute

3:00pm **2D+EM+MN+NS-ThA3 Optospintronics and Magnetism with 2D Materials and Heterostructures**, ***Roland Kawakami,*** The Ohio State University **INVITED**

I will review our latest developments in spintronics, optospintronics and magnetism in two-dimensional (2D) materials and heterostructures. Graphene continues to exhibit improved properties for spin transport and demonstrates additional functionality through the use of vertically stacked heterostructures. One of the interesting new directions is optospintronics enabled by heterostructures of graphene and transition metal dichalcogenides (TMD) [1]. Due to the valley optical selection rules of TMDs and the large spin-orbit coupling, the helicity of the photon is coupled to the valley spin polarization of electrons. Thus, circularly polarized optical excitation into a TMD/graphene heterostructure generates spin polarization in the TMD that subsequently transfers to the graphene. This optical spin injection into graphene is an example of new functionality for the expanding field of 2D spintronics. In the area of 2D magnets, we have used molecular beam epitaxy (MBE) to deposit monolayer $MnSe_2$, which exhibits ferromagnetism at room temperature [2]. These results open the door for new possibilities for magnetoelectronic applications with low dimensional materials.

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4:00pm **2D+EM+MN+NS-ThA6 Giant Electromechanical Response in Van-der-Waals Layered Crystals**, ***Sabine Neumayer***, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory; *E.A. Eliseev,* National Academy of Sciences of Ukraine; *A. Tselev,* CICECO and Department of Physics, University of Aveiro, Portugal; *A.N. Morozovska,* National Academy of Sciences of Ukraine; *M.A. Susner, M.A. McGuire,* Oak Ridge National Laboratory; *J. Brehm, S. Pantelides,* Vanderbilt University; *N. Balke, P. Maksymovych,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Obtaining ultrathin electromechanically active materials for memory and energy applications encounters numerous challenges as significant downscaling of classical ferroelectrics such as perovskite oxides is severely constrained by size and screening effects. Moreover, interfacing pseudo-cubic ferroelectrics with 2D electronic materials faces challenges related to defect and impurities, which limit performance. Van der Waals ferroelectrics, especially transition metal thiophosphates such as copper indium thiophosphate (CIPS) yield promising prospects for applications as ultrathin piezoelectric structures and interface materials due to their stable surfaces, layered structure and transition temperatures near room temperature. Here, we use scanning probe microscopy to explore the remarkable functional properties of CIPS across the transition temperature. At low temperatures, strong electromechanical response is measured despite the small polarization values and the material contracts in electric fields rather than expanding. These findings point to giant negative electrostrictive coefficients, which were quantified using Landau-Ginzburg-Devonshire analysis. Above the transition temperature, CIPS shows dielectric tunability comparable to BST at low frequencies. In addition, electromechanical strain exceeding 10 nm displacement was measured upon fully reversible field induced formation of particles on the surface. Complimentary DFT calculations provide further insight into the role of ionic displacement in electromechanical behavior.

Research conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility . Research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

4:20pm **2D+EM+MN+NS-ThA7 A Universal Method for Measuring Valleytronic Quality of 2D Materials using Conventional Raman Spectroscopy**, ***Steven Vitale***, *J.O. Varghese, D.A. Nezich, M. Rothschild,* MIT Lincoln Laboratory

Valleytronics offers a new information processing paradigm based on the momentum index of real or quasi-particles in 2D materials as the fundamental unit of information storage instead of charge. A major challenge to realize valleytronic computing is the development of deterministic material growth processes which yield valleytronic-quality material with the requisite valley relaxation lifetime (T1) and valley dephasing time (T2). Unfortunately direct measurement of T1 and T2 requires complex instrumentation to perform ultrafast spectroscopic measurements and thus is not practical for routine material analysis. In this paper, we demonstrate that an accurate and reproducible measurement of $T1/T_{exc}$ (where T_{exc} is the exciton recombination lifetime) can be performed a simple Raman microscope. By simultaneously measuring the photoluminescence of the 2D material and the Raman transition of the underlying silicon substrate as a function of the incident laser polarization angle, one can remove sources of error and equipment-to-equipment variability. This technique is completely general and can be applied to any

valleytronic material which can be grown-on or transferred-to a Raman-active crystalline substrate, such as silicon. Using this technique we show that valley relaxation in a sample of CVD-grown MoS_2 is an order of magnitude slower at 4 K than at 100 K. Oxidation of MoS_2 left exposed to the ambient environment severely decreases the valleytronic quality of the material. Two-dimensional mapping of the valley relaxation time of CVD MoS_2 domains at 4 K shows a three-fold spatial symmetry which is suggestive of new valley physics phenomena which arise in 2D crystals of finite size. MoS_2 domain size also affects the valley relaxation time, which has significant material-growth implications for real valleytronic applications. Finally we compare these measurements to our calculated requirements for valley relaxation time in a practical information processing device and quantify the challenges for future valleytronic material growth.

4:40pm **2D+EM+MN+NS-ThA8 Discovery of Intrinsic Ferromagnetism in 2D van der Waals Crystals**, ***Xiang Zhang***, *C. Gong,* University of California, Berkeley **INVITED**

In this talk, I will present our discovery of the intrinsic ferromagnetism in 2D van der Waals (vdW) crystals, including the prominent dimensionality effect and unprecedented magnetic field control of the Curie temperature in the nearly-ideal 2D Heisenberg ferromagnet. Significant fundamental physics in 2D magnetism and the corresponding exotic phenomena we observed will be expounded. Updated research on the complex magnon scatterings, material level engineering of 2D magnetism, and the development of novel concept of spintronic devices will be further discussed. Finally, I will envision the possible directions towards advancing 2D magnets for practical spintronic applications.

5:20pm **2D+EM+MN+NS-ThA10 Spectroscopic Evidence of Pair-mediated Bosonic Modes in Superconductor FeSe/$SrTiO_3$(100) Film**, ***Minjun Lee***, Seoul National University, Republic of Korea*; M. Oh, H. Jeon, S. Yi, I. Zoh,* Seoul National University, Republic of Korea*; C. Zhang,* Seoul National University, Republic of Korea*; J. Chae, Y. Kuk,* Center for Quantum Nanoscience, Institute for Basic Science, Republic of Korea

Single layer FeSe on $SrTiO_3$(100) is atypical but noticed system in superconductivity. This has unique properties due to the substrate phonon. Unlike other bulk systems, the presence of the interface allows the substrate phonons to affect the superconducting layer. We have investigated substrate phonon effects on superconducting FeSe layer by using scanning tunneling spectroscopy and Eliashberg theory. We were able to measure acoustic, optical and substrate phonons in d^2I/dV^2 spectroscopy. We found these phonon modes attribute to the paring of electrons in this superconducting layer. These results are analyzed by Eliashberg model and we will discuss the coupling strength of these bosonic features. We have found that the substrate phonon has major contribution to increase the transition temperature of this system.

Electronic Materials and Photonics Division
Room 101A - Session EM+2D+NS+PS+RM+TF-ThA

IoT Session: Flexible Electronics & Flash Networking Session

Moderators: Shalini Gupta, Northrop Grumman ES, Sang M. Han, University of New Mexico

2:20pm **EM+2D+NS+PS+RM+TF-ThA1 Epitaxial Electrodeposition of Electronic and Photonic Materials onto Wafer-size Single Crystal Gold Foils for Flexible Electronics**, ***Jay Switzer***, Missouri University of Science and Technology **INVITED**

Single-crystal silicon (Si) is the bedrock of semiconductor devices due to the high crystalline perfection that minimizes electron-hole recombination, and the dense SiO_x native oxide that minimizes surface states. There is interest in moving beyond the planar structure of conventional Si-based chips to produce flexible electronic devices such as wearable solar cells, sensors, and flexible displays. Most flexible electronic devices are based on polycrystalline materials that can have compromised performance due to electron-hole recombination at grain boundaries. In order to expand the palette of electronic materials beyond planar Si, there is a need for both an inexpensive substrate material for epitaxial growth, and an inexpensive and scalable processing method to produce epitaxial, grain-boundary-free films of metals, semiconductors, and optical materials. Recently, in our laboratory, we have developed a process for producing wafer-size, flexible, and transparent single-crystal Au foils by an electrochemical processing method.[1] Au is epitaxially electrodeposited onto Si using a very negative applied potential. An interfacial layer of SiO_x is then produced photoelectrochemically by lateral undergrowth. The Au foil is then removed by epitaxial lift-off following an HF etch. We will report on the electrodeposition of epitaxial films of metal oxide semiconductors such as Cu_2O and ZnO onto the highly-ordered and flexible Au foils. We will also present new, unpublished results in which we spin-coat epitaxial films of perovskites, such as $CsPbBr_3$, directly onto these Au foils and onto other single crystals.

Acknowledgement: This presentation is based on work supported by the U.S. Department of Energy, Office of Basic Sciences, Division of Materials Science and Engineering under grant No. DE-FG02-08ER46518.

[1] Mahenderkar N., Chen Q., Liu Y.-C., Duchild, A., Hofheins, S. Chason E., Switzer J (2017). Epitaxial lift-off of electrodeposited single-crystal gold foils for flexible electronics. Science, **355**, 1203-1206.

3:00pm **EM+2D+NS+PS+RM+TF-ThA3 Flexible Electronic Devices Based on Two Dimensional Materials**, *R. Kim, N.R. Glavin,* Air Force Research Laboratory*; R.H. Rai, K. Gliebe, M. Beebe,* University of Dayton; Air Force Research Laboratory*; J. Leem, S. Nam,* University of Illinois at Urbana-Champaign*; R. Rao,* Air Force Research Laboratory*;* ***Christopher Muratore***, University of Dayton*; K.M. Burzynski,* University of Dayton and Air Force Research Laboratory, Materials and Manufacturing Directorate

Low temperature synthesis of high quality 2D materials directly on flexible substrates remains a fundamental limitation towards realization of robust, strainable electronics possessing the unique physical properties of atomically thin structures. Here, we describe room temperature sputtering of uniform, stoichiometric amorphous MoS_2, WSe_2, and other transition metal dichalcogenides and subsequent large area (>2 cm^2) photonic crystallization to enable direct fabrication of two-dimensional material photodetectors on large area flexible PDMS substrates. Fundamentals of crystallization kinetics for different monolithic and heterostructured TMDs are examined to evaluate this new synthesis approach for affordable, wearable devices. The photodetectors demonstrate photocurrent magnitudes and response times comparable to those fabricated via CVD and exfoliated materials on rigid substrates and the performance is unaffected by strains exceeding 5%. Other devices and circuits fabricated from crystallized 2D TMDs deposited on large area flexible substrates are demonstrated.

3:20pm **EM+2D+NS+PS+RM+TF-ThA4 Contact Resistances and Schottky Barrier Heights of Metal-SnS Interfaces**, ***Jenifer Hajzus***, *L.M. Porter,* Carnegie Mellon University*; A. Biacchi, S. Le, C. Richter, A. Hight Walker,* National Institute of Standards and Technology (NIST)

Tin(II) sulfide (SnS) is a natively p-type, layered semiconductor that is of interest for two-dimensional and optoelectronic applications. Understanding the behavior of contacts to SnS is essential for its use in devices. In this work, contact metallizations with a range of work functions were characterized on both solution-synthesized, p-type SnS nanoribbons and electron-beam evaporated, polycrystalline SnS thin films. The structure and properties of electron-beam evaporated SnS films were dependent upon deposition temperature and post-deposition annealing. A deposition temperature of 300 °C followed by vacuum annealing at 300 °C resulted in p-type, orthorhombic SnS films. Specific contact resistances of Ti/Au, Ru/Au, Ni/Au, and Au contacts were measured on SnS films using circular transfer length method (CTLM) patterns prior to and after annealing the contacts at 350 ° C in argon. All metallizations on SnS thin films were ohmic prior to annealing. A trend of decreasing average specific contact resistance with increasing metal work function was observed for the as-deposited contacts. Annealed Ru/Au exhibited the lowest average specific contact resistance of ~1.9 x 10^{-3} Ω -cm^2. Contacts were additionally patterned onto individual, solution-synthesized SnS nanoribbons. In contrast to the behavior of contacts on electron-beam evaporated films, low work function metals (Cr/Au and Ti/Au) formed Schottky contacts on SnS nanoribbons, whereas higher work function metals (Ni/Au and Pd/Au) formed ohmic or semi-ohmic contacts. Ni/Au exhibited a lower contact resistance (~10^{-4} Ω cm^2 or lower) than Pd/Au (~10^{-3} Ω cm^2 or lower). Schottky barrier heights and ideality factors of Cr/Au and Ti/Au contacts were extracted by fitting current-voltage measurements to a back-to-back Schottky diode model. The ohmic behavior for Ni/Au and Pd/Au and the calculated Schottky barrier heights (0.39 and 0.50 eV for Cr/Au and Ti/Au, respectively) on SnS nanoribbons agree well with behavior predicted by Schottky–Mott theory and suggest a lack of Fermi level pinning.

MEMS and NEMS Group
Room 202B - Session MN+2D+AN+NS-ThA
Nonlinear and Thermal Resonators

Moderators: Meredith Metzler, University of Pennsylvania, Christian Zorman, Case Western Reserve University

2:20pm **MN+2D+AN+NS-ThA1 Embracing Nonlinearity and Thermal Fluctuations in Nanomechanics**, *D. Lopez, **David Czaplewski**, C. Chen,* Argonne National Laboratory*; D. Zanette,* Centro Atomico Bariloche, Argentina*; S. Shaw,* Michigan State Univrsity **INVITED**

The field of micro-mechanics is now a well-established engineering domain with demonstrated impact in fundamental science and product development. Unfortunately, as the dimensions of the devices are reduced from the micro- to the nano-scale, the direct scaling of the fundamentals principles and fabrication processes cease to work. When going from micro- to nano-mechanical systems, MEMS to NEMS, the devices linear dynamic range can be reduced to the point where the amplitudes needed for lineal response are below the noise level and, as a consequence, operation in the nonlinear regime is unavoidable. Furthermore, thermal fluctuations and fluctuation-induced forces become relatively stronger causing significant changes in their dynamic response and on the manner in which they interact with the surrounding environment. This combination of nonlinear dynamics and high sensitivity to fluctuations has been seen as a deleterious combination for the advance of nano mechanical devices.

Rather than continuing to struggle to avoid these phenomena, it is of interest to consider how micro/nanosystem might effectively capitalize on this nonlinear fluctuating response. In this talk, I will demonstrate that nonlinearity offers unique possibilities for the controlled response of micro and nano mechanical devices and, thereby, a host of novel application opportunities. Examples of these opportunities include the development of compact frequency sources with low phase noise, the engineering of dissipation reservoirs to manipulate energy decay processes, and the enhancement of synchronization range between microscopic and macroscopic oscillators.

3:00pm **MN+2D+AN+NS-ThA3 Probing Ion Radiation Effects in Silicon Crystals by 3D Integrated Resonating Thin Diaphragms**, ***Hailong Chen**, H. Jia, V. Pashaei,* Case Western Reserve University*; W. Liao, C.N. Arutt, M.L. McCurdy,* Vanderbilt University*; P. Hung,* The Aerospace Corporation*; R.A. Reed, R.D. Schrimpf, M.L. Alles,* Vanderbilt University*; P.X.-L. Feng,* Case Western Reserve University

Space radiation (*e.g.*, solar, galaxy) and man-made radiation environments (*e.g.*, nuclear plant) can expose devices to radiation at doses that may lead to severe damage [1]. In recent decades, a large body of work has been performed to understand radiation effects on mainstream solid state electronic devices [1-3], in particular on MOS devices [2] and integrated circuits [3]. Lately, microelectromechanical systems (MEMS) have seen widespread adoption in consumer, military and aerospace products due to their small size, low power consumption, and in some cases, monolithic integration with electronics [4]. As such, the reliability of MEMS devices for many applications in relatively benign environments has been well established [5]. However, the study of impact on mechanical properties due to radiation-induced damages is an area where limited research has been conducted.

In this work, we report on experimental investigation of heavy ion radiation effects on mechanical properties of Si crystals, by exploiting a novel 3D scheme of using 5 vertically stacked micromachined vibrating Si diaphragms (2 mm × 2 mm x 2 µm) exposed to oxygen ions. Simulations find the stop range of oxygen ions in Si is 7.3 µm. A Pelletron system is employed to irradiate oxygen ions into the Si diaphragms (10.3MeV, with a dose of 5.6 $\times 10^{13}/cm^2$). Before and after radiation, multimode resonances are characterized in vacuum by using an ultrasensitive optical interferometry system. We have observed that diaphragms D1 and D2, which oxygen ions are expected to pass completely through, present modest multimode redshifts ranging from 0.85 kHz to 1.67 kHz, and 0.85 kHz to 1.19 kHz, corresponding to an average fractional frequency shift of 10.5% and 7.0%, respectively. In contrast, for devices D3 and D4, in which most ions are expected to stop, each resonance peak shifts much more dramatically, with a frequency shift of 27.3% and 20.4%. We attribute these large shifts to the very large capture area of the diaphragms, the very heavy and energetic oxygen ions, and high ion dose. Device D5 shows minimal frequency shifts among the five diaphragms because few oxygen ions reach and interact with this device layer. The diaphragm stack exhibits outstanding capability for probing radiation damages in MEMS, not only able to capture the radiation events obviously, but also help analyze different amount and types of damages induced in each stacking layer.

[1] L. Gregory, *et al.*, Proc. IEEE. **62**, 1974. [2] J. R. Srour, *et al.*, Proc. IEEE. **76**, 1988. [3] H. L. Hughes, *et al.*, IEEE Trans. Nucl. Sci. **50**, 2003. [4] N. Arutt, *et al.*, Semicond. Sci. Technol. **32**, 2017. [5] H. R. Shea, Proc. SPIE. **7928**, 2011.

3:20pm **MN+2D+AN+NS-ThA4 An Array of Thermally-actuated Nanoresonators for Real-time Mass Spectrometry**, ***Martial Defoort**, M. Sansa, M. Gély, G. Jourdan, S. Hentz,* CEA/LETI-University Grenoble Alpes, France

Micro/Nano-ElectroMechanical Systems (M/NEMS) have attracted much attention in the last years in the mass spectrometry field. They feature high sensitivity, charge independent and single particle detection capabilities, in a mass range where conventional mass spectrometry struggles, hampering the analysis of large mass objects like protein complexes or viruses [1-4].

In general the size and mass of the device defines the size and mass ranges of the particles to measure for frequency tracking and point mass approximation purposes. However, as many silicon M/NEMS are electrostatically actuated, the gap between the driving electrode and the resonator becomes a critical parameter. While for many applications this gap should be as small as possible for high efficiency actuation and high signal-to-noise ratio, a particle landing within the gap results in a catastrophic failure of the device through electrical short-circuit or mechanical anchoring.

We present a new actuation scheme for doubly-clamped beams which rel ies on the thermal expansion of nano-actuators in silicon due to Joule heating, located close to the anchor of the resonator (Fig. 1), that we demonstrate to work in an array of 20 NEMS (Fig. 2). Unlike some thermoelastic actuation schemes [5], the technique we propose does not require an additional layer (of, for example, a metal) and is readily CMOS-compatible. Because of their small size and thermal capacity, the thermal time constant of the actuators is small enough to drive the resonator up to several 100's MHz with large efficiency and to actuate the two first flexural modes of the same device simultaneously, which is required for single particle mass sensing . The detection scheme uses the piezoresistive gauges located on the other end of the beam, as previously presented [6]. We compare the performance of this actuation technique with a standard electrostatic scheme both on the same array and demonstrate the thermal actuation does not affect the level of frequency fluctuations limiting the device mass resolution (Fig. 3).

1. Hanay *et al*, nature nanotechnology 2012.

2. Sage *et al*, nature communications 2015.

3. Sage *et al*, Arxiv 2017.

4. Dominguez-Medina *et al*, Arxiv 2018.

5. Mo Li *et al*, nature nanotechnology 2007.

6. Mile *et al*, nanotechnology 2010.

4:00pm **MN+2D+AN+NS-ThA6 Nonlinear and Noise Induced Dynamics of High Q Nanomechanical Resonators**, ***Jana Huber**, E.M. Weig,* University of Konstanz, Germany **INVITED**

Doubly-clamped pre-stressed silicon nitride string resonators excel as high Q nanomechanical systems enabling room temperature quality factors of several 100,000 in the 10 MHz eigenfrequency range when operated under vacuum conditions. To retain the high mechanical quality factor, dielectric transduction is implemented as an all-electrical control scheme avoiding the metallization of the string. To this end, the string is exposed to an inhomogeneous electric field created between adjacent electrodes. The resulting gradient field provides an ideal platform for actuation, displacement detection, frequency tuning as well as strong mode coupling between the in- and out-of-plane modes of the string.

Here we focus on the nonlinear dynamics of the string subject to a strong drive. As a result of the high quality factor, cubic as well as higher order nonlinearities are observed. In the presence of thermal fluctuations, satellite resonances arise which enable deep insights into fundamental properties of the system.

4:40pm **MN+2D+AN+NS-ThA8 A Buckling-based, DC Controlled, Non-volatile Nanoelectromechanical Logic Memory**, *S.O. Erbil, **Utku Hatipoğlu**,* Bilkent University, Turkey*; C. Yanık,* Sabancı University*; M. Ghavami, M.S. Hanay,* Bilkent University, Turkey

Here, we demonstrate a buckling based, nanoelectromechanical logic bit with high controllability and low logic input voltage. The device consists of

a slender beam to store information through its buckling direction and a comb-drive structure for initiating buckling electrostatically. When an actuation voltage is applied to the fingers of the comb-drive structure, an axial compressive force is applied to the suspended slender beam which is connected to an anchor from the opposite end. Applied axial force creates a compressive stress on the slender beam which leads to buckling after a critical load. Buckling direction can be controlled (left/right) by changing the applied side-gate control voltages. The capacitive attraction force generated between the beam and the activated electrode controls the direction of the buckling. Control voltage acts as the logic input for writing information and it is only required just before the application of the axial load, so that the beam can be preloaded to the target direction. Lateral deformations as large as 10% of the beam length can be achieved.

Once the beam is buckled to the desired direction, the removal of the guidance voltage does not affect the buckling state of the beam, which indicates successful non-volatile information storage. Moreover, by altering the voltage difference created in the comb-drive structure, buckling amount can be controlled very precisely. Control voltages as low as 0.5V are demonstrated for storing information. The device is fabricated from an SOI wafer by using electron beam lithography, metal deposition and plasma / HF etching techniques. The dimensions of the slender beam are 150nm x 250nm x 40µm for the width, thickness and length respectively. Several videos demonstrating dynamically controlled electrostatic buckling have been recorded during the experiments. The nanoelectromechanical logic memory demonstrated here is scalable since its operation does not require any high-end electronic instruments such as function generators, and can be accomplished by simply using DC power sources. To readout the state of the beam all-electronically, the device is capacitively coupled to a microwave resonator. The changes in the frequency shows clear transitions between buckled and straight states.

It is possible to build two-bit mechanical logic gates and more involved logic units by using proposed nanoelectromechanical logic bit. As a further matter, precise control of the buckling in nanoscale can be very promising for demonstrating the interconnection between information science and thermodynamics.

Nanometer-scale Science and Technology Division
Room 102B - Session NS+2D+AS+MN+PC-ThA

SPM – Probing Electronic and Transport Properties

Moderators: Ondrej Dyckoe, Oak Ridge National Laboratory, Sergei Kalinin, Oak Ridge National Laboratory, Indira Seshadri, IBM Research Division, Albany, NY

2:20pm **NS+2D+AS+MN+PC-ThA1 Imaging Currents in Two-dimensional Quantum Materials**, ***Katja Nowack,*** Cornell University **INVITED**

Magnetic imaging is uniquely suited to the non-invasive imaging of current densities, particularly in two-dimensional devices. In this talk, I will showcase this approach by discussing measurements on HgTe quantum well devices in the quantum spin Hall (QSH) regime. In a nutshell, we scan a superconducting quantum interference device (SQUID) to obtain maps of the magnetic field produced by the current flowing in a device. From the magnetic image we reconstruct a two-dimensional current distribution with a spatial resolution on the micron scale. This allows us to directly visualize that most of the current is carried by the edges of the quantum well devices when tuned into their insulating gaps - a key feature of the QSH state. I will both discuss routes towards improving the spatial resolution of our measurements to sub-micron length scales through a combination of improved image reconstruction and smaller sensor sizes.

3:00pm **NS+2D+AS+MN+PC-ThA3 Side-gate Construct for Probing Active Energy Levels in Electron Transport through a Solid-state Surface-bound Protein Monolayer**, ***Sidney Cohen,*** *B. Kayser, C. Gua, M. Sheves, I. Pecht, D. Cahen,* Weizmann Institute of Science, Israel

Electron transport studies provide an excellent platform to deduce electronic structure in molecular electronics studies, enabling control and understanding of the pathways and mechanisms involved. Due to their complexity, proteins are used only infrequently in this context, despite convenient properties such as selective binding, self-assembly, light sensitivity, and the possibility to (bio) chemically tailor properties . Here, we study electron transport in monolayer films of Azurin, using a 3-electrode configuration with a novel side-gate. The source and drain are gold substrate and conductive atomic force microscope (C-AFM) probe, respectively. The measuring devices were prepared in a two-step electron beam lithography process, whereby interdigitated drain and gate electrodes with separation of 80 nanometers are patterned from macroscopic electrodes, the latter formed optically on a silicon oxide substrate. The gold electrodes are patterned with the gate elevated by 20 nm for improved coupling with the drain. After deposition of the Azurin monolayer on this structure, the carrier chip was wire-bonded for insertion into the AFM. Azurin was incorporated in the device both as copper-containing holo-Azurin, and as apo-Azurin with the Cu ion removed. Stability of source-drain vs. $V_{source\text{-}drain}$ curves, as well as gate-drain leakage were monitored for validity. $I_{source\text{-}drain}$ vs. $V_{source\text{-}drain}$ curves were acquired at different gate voltages, and $I_{source\text{-}drain}$ at 0 $V_{source\text{-}drain}$ was measured while sweeping V_{gate} in both polarities. Asymmetry of current onset for opposing gate biases points to a low-lying LUMO transport level for holo-Azurin. For apo-Azurin this level is shifted to higher values and hence inaccessible. Semi-quantitative location of the tail of this LUMO, as well as value of gate coupling were estimated by changing the work function of the drain electrode, i.e. C-AFM probe, from Pt (ϕ=-5.3 eV) to Au (ϕ= -4.9 eV). The observations can be rationalized by considering previous electrochemical and theoretical studies.

3:20pm **NS+2D+AS+MN+PC-ThA4 Adding Electrons One at a Time to Electrostatically Confined Graphene Quantum Dots**, ***Daniel Walkup,*** *C. Gutierrez, F. Ghahari,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; C. Lewandowski,* MIT*; J. Rodriguez-Nieva,* Harvard University*; T. Taniguchi, K. Watanabe,* National Institute for Materials Science (NIMS), Japan*; L. Levitov,* MIT*; N.B. Zhitenev, J.A. Stroscio,* National Institute of Standards and Technology (NIST)

The Coulomb blockade of adding charges to isolated metallic systems is one of the most characteristic phenomena of quantum dots (QDs). Here, we created circular graphene QDs in a backgated graphene-hexagonal boron nitride (hBN) device by locally ionizing defects in the hBN layer, using the electric field from the tip of a scanning tunneling microscope (STM). Scanning tunneling spectroscopy (STS) enables us to image the local density of states outside and within these circular graphene resonators. At weak magnetic fields, confinement of graphene electrons is poor and Coulomb blockade is not observed. At higher fields, however, the graphene electrons form quantized Landau levels (LLs) separated by energy gaps. In the area of the QD, the LLs are bent by the electrostatic potential creating metallic (compressible) rings where a LL crosses the Fermi energy, separated by circular insulating barriers (incompressible strips), which isolate the dot from the graphene and enable the onset of Coulomb blockade. Tunneling dI/dV spectra inside the QD reveal a series of Coulomb blockade peaks, which shift as a function of back gate voltage. In the plane defined by gate voltage and sample bias, these peaks form Coulomb lines, whose slope is governed by the relative capacitances between the dot, tip, gate, and sample bias electrodes, and whose relative offsets reveal the addition spectrum of the quantum dot. A characteristic feature of the Coulomb blockade in these systems is the presence of different families of charging lines, one for each LL, which intersect each other and experience avoided crossings. The avoidance pattern of these anticrossings is novel: at the strongest fields, it somewhat resembles the predictions of simple models of electrostatically-coupled QDs, but at weaker fields it diverges very strikingly, and new modeling is needed to reproduce it. This avoidance pattern reflects the interaction of electrons in different LLs, occupying different parts of the QD, and is tunable via the magnetic field and gate voltage. By moving the STM tip, we can tune the tip-dot capacitance, and tunnel into different parts of the dot, enabling a full characterization of the anticrossings in these novel electronic nanostructures.

4:00pm **NS+2D+AS+MN+PC-ThA6 Bulk and Surface Contribution to the Charge and Spin Transport in Topological Insulators Observed with a Four-Probe Scanning Tunneling Microscope**, ***Wonhee Ko,*** *G.D. Nguyen,* Oak Ridge National Laboratory*; H. Kim, J.S. Kim,* Pohang University of Science and Technology, Republic of Korea*; A.-P. Li,* Oak Ridge National Laboratory

Topological insulators are fascinating materials for future electronics because of its superior charge and spin transport characteristics stemming from their topological nature. However, topological insulators realized in actual materials have both bulk and surface carriers, where the former significantly hampers the topological transport of the later. In this talk, we utilize four-probe scanning tunneling microscope to investigate bulk and surface contribution to the charge and spin transport in bulk-insulating topological insulator Bi_2Te_2Se. The relative contribution of bulk and surface was varied by changing temperature and transport area, which was measured by variable probe-spacing spectroscopy. The surface dominant regime was already reached at 82 K, where the sample exhibited superior

transport properties such as a large surface mobility and high spin polarization. At this regime, the contact to external probes also transforms from Schottky to Ohmic junction. Our result indicates that controlling bulk and surface contribution to the transport is crucial for realizing topological devices.

4:20pm **NS+2D+AS+MN+PC-ThA7 Modulation of Single-Walled Carbon Nanotube Electronic Structure by External Electronic Perturbations: Scanning Tunneling Spectroscopy and Density Functional Theory**, ***Benjamen Taber***[1], *G.V. Nazin,* University of Oregon

Understanding the local impact of environmental electronic perturbations on the local density of states (LDOS) of single-walled carbon nanotubes (CNTs) is critical for developing CNT-based devices. We present scanning tunneling microscopy and spectroscopy (STM/STS) investigations of CNTs adsorbed on both a metal, Au(111), and a dielectric, monolayer RbI on Au(111), serving as models for stronger and weaker electrostatic interactions, respectively. In both cases, STS revealed modulations in the CNT LDOS corresponding to features in the underlying material. We then corroborate our STM/STS results with density functional theory calculations of the electronic structure of semiconducting CNTs in the presence and absence of an external dipole (a pair of opposite charges). DFT-calculated CNT LDOS quantitatively matched STM/STS results, providing key insight in to the local impact external charges have on CNT electronic structure.

4:40pm **NS+2D+AS+MN+PC-ThA8 Single Charge and Exciton Dynamics probed on the Molecular Scale**, ***Anna Roslawska***, *P. Merino, C. Grosse, C.C. Leon, O. Gunnarsson, M. Etzkorn, K. Kuhnke, K. Kern,* Max Planck Institute for Solid State Research, Germany

The performance of organic optoelectronic devices depends on the dynamics of charges and excitons (electron-hole pairs). The relevant processes have been mostly studied by time-resolved techniques with a spatial resolution limited by optical diffraction. In order to overcome this limit, a nanoscale scanning probe approach that enables addressing individual light emitters is preferred. Here we introduce time-resolved scanning tunneling microscopy-induced luminescence (TR-STML) and use it to explore locally the single charge and single exciton regime. The excitonic light originates from structural defects in C_{60} thin films on Au(111) that act as charge and exciton traps. Such a defect is a single photon emitter, whose spectrum has a sharp electron-hole recombination feature [1,2]. By measuring the time-resolved electroluminescence due to individual injected charges, it is possible to analyze the formation and recombination processes of single excitons and determine their characteristic time constants[3].

[1] P. Merino, C. Große, A. Rosławska, K. Kuhnke, K. Kern, , Nat. Commun., 6, 8461, 2015.

[2] C. Große, P. Merino, A. Rosławska, O. Gunnarsson, K. Kuhnke, K. Kern, ACS Nano, 11, 1230-1237, 2017.

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5:00pm **NS+2D+AS+MN+PC-ThA9 Microscopic Understanding of the Temperature-dependent Carrier Transport in Ge Nano - Crystal s Films**, ***Dan Shan***, Yangzhou Polytechnic Institute, China*; J. Xu,* Nanjing Universityy, China

Silica-based semiconductor nano-crystals have attracted much interest in recent years due to their possible applications in many kinds of nano-electronic and optoelectronic devices. Compared with Si, Ge has larger electron and hole mobility. Furthermore, Ge has a narrower band-gap and high phonon responsivity in the near-infrared region, so it is suited to many near-infrared applications. In order to further improve the device performance, detailed knowledge of transport mechanisms across these nano-crystals becomes necessary and is considered indispensable.

In this work, hydrogenated amorphous germanium films were prepared by a plasma enhanced chemical vapor deposition technique. Ge nano-crystals (Ge NCs) films were obtained by thermal annealing the as-deposited samples. P-type behavior in Ge NCs films without any external doping is attributed to the holes accumulation caused by acceptor-like surface states. It can be found that the dark conductivity and Hall mobility reach to as high as 25.4 S/cm and 182 $cm^2/V{\cdot}s$ in the Ge NCs film, which are much higher than the previously reported data. Carrier transport mechanisms of Ge NCs films were investigated by temperature-dependent Hall measurement. Three kinds of temperature-dependent conductivity behaviors, which exhibit the linear relationships of the ln σ versus $T^{-1/4}$, $T^{-1/2}$ and T^{-1}, respectively, were observed in the temperature regions of 10-500 K. It can be confirmed that the thermal activation conduction in the extended states dominated the carrier transport process above 300 K (300-500 K). Below room temperature, the carrier transport process was dominated by the percolation-hopping conduction at 90-230 K and turned to Mott-VRH conduction when the temperature falling below 50 K (10-50 K).

Furthermore, the different scattering mechanisms in carrier transport process were found in different temperature regions, which were evaluated via temperature-dependent Hall mobilities. In the low temperature region (10-50 K), the carrier Hall mobility is almost temperature independence ($\mu \sim T^0$), revealing the neutral impurities' scattering mechanism dominated the carrier transport process. When increasing the temperature (50-190 K), the carrier transport properties were controlled by the grain boundary scattering mechanism, where the carrier Hall mobility was increased with temperature and exhibited the thermally activated behavior. However, the relationship of $\mu \sim T^{-0.9}$ was observed above room temperature (300-500 K). It is suggested that the carrier transport is dominated by a superposition of grain boundary scattering and acoustic phonon scattering within the high temperature region.

[1] **NSTD Postdoc Finalist**

2D Materials Focus Topic
Room Hall B - Session 2D-ThP
2D Materials Poster Session

2D-ThP1 Activated Reduction Plasma Assisted Sulfurization in Layered WS_2 Synthesis, ***Chien-Pao Lin**, C.-N. Hsiao,* ITRC,NARL, Taiwan, Republic of China*; P.-S. Chen, C.-A. Jong,* No Matching Affiliation, Taiwan, Republic of China

CVD process is known as a promising method in large domain size and continuous 2D film synthesis. Sulfurization of Group VIB contained precursor (metal or metal oxide) for sulphide formation were widely studied. Sulfur is also reported as reduction agent of metal oxide at initial stage. In some cases, H_2 flew along with sulfur vapor during reduction time in MOCVD [1] and ALD [2] process. H_2 could be beneficial in the impurity removal and to enlarge the domain size effectively.

Plasma source in vacuum technology is useful especially in lowering the process temperature and for increasing the precursor decomposition efficiency in CVD or ALD process. R. Morrish et al., revealed that a and longer than 30 min at 500°C for sulfurization process using 10% H_2S plasma could reduce the activation energy between WO_3 and H_2S [3]. The presence of energetic radicals such as atomic S and H during sulfurization, the temperature and the exposure time are important.

In this study, we demonstrated the sulfurization process by two steps: (1) The energetic hydrogen (H*) generated by ICP plasma in WO_3 reduction at early stage, (2) Reaction between the activated hydrogen (H*) and sublimated sulfur vapor for WS_2 formation. The hydrogen concentration, plasma exposure time, the reaction temperature and duration time are evaluated for the sulfurization of WO_3.

WO_3 film was deposited on Si substrate covered by 90 nm thermal dry oxide. Samples were sulfurized in a 4 inch inductively coupled plasma (ICP) reactor with copper coil connected to a 13.56 MHz RF power supply. The reaction temperature varied from 700 to 900°C. Raman and PL spectrum were adopted for the film quality inspection. The surface roughness of formed WS_2 layers were examined by AFM. The best condition performed when the reaction temperature was 850°C with 5% H_2 plasma pre-treatment for 20min. Higher H% is harmful for film formation, which was similar to the report by K. N. Kang et al. that sulfurization can etch the damage of the film [4]. Raman and photoluminescence (PL) spectroscopy were taken with 532 nm excitation. The uniform Raman signals and PL spectrum within 4 cm^2 are shown and the center of the PL peak was at 629 nm (1.97 eV).

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2D-ThP2 Quantized States, Berry Phases, and Quantum-Hall Wedding-Cake structures in Graphene Quantum Dots, ***Fereshte Ghahari Kermani**, D. Walkup, C. Gutiérrez,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; C. Lewandowski,* Department of Physics, Massachusetts Institute of Technology*; J. Rodriguez-Nieva,* Massachusetts Institute of Technology*; K. Watanabe, T. Taniguchi,* National Institute for Materials Science, Japan*; L. Levitov,* Massachusetts Institute of Technology*; N.B. Zhitenev, J.A. Stroscio,* National Institute of Standards and Technology (NIST)

Recent progress in creating and probing graphene quantum dots (QDs) with fixed build-in

potentials has offered a new platform to investigate Klein tunneling related phenomena . In this talk, I describe scanning tunneling spectroscopy measurements of the energy spectrum of graphene QDs as a function of energy, spatial position, and magnetic field. In the absence of a magnetic field, confinement of graphene carriers in a *p-n* junction resonator gives rise to a series of quasi-bound single particle states which result from oblique Klein scattering at the *p-n* interface. Applying a weak magnetic field, we observe a giant and discontinuous change in the energy of time-reversed angular-momentum states, which manifests itself as the appearance of “new” resonances in the tunneling density of states. This behavior corresponds to the on/off switching of a π- Berry phase when a weak critical magnetic field is reached. With increased applied magnetic field, the QD states can be confined even further as they condense into highly degenerate Landau levels providing the first spatial visualization of the interplay between spatial and magnetic confinement. This is observed as formation of the seminal wedding-cake structures of concentric compressible and incompressible density rings in strong magnetic fields.

2D-ThP3 Growth Phenomena and Mechanism of MoS2 Formed by Conventional Chemical Vapor Deposition, ***Cheol-Min Hyun**, J.H. Choi, S.W. Lee, J.-H. Ahn,* Korea Maritime and Ocean University, Republic of Korea

In recent years, transition metal dichalcogenide (TMDC) compound, have heen studied as a platform for next generation semiconductor devices. One of the most representative two-dimensional TMDC materials, MoS2 is applied as a device as well as various synthesis methods are known, including chemical vapor deposition. However, in-depth research on the synthesis process and the mechanism of the variable has not been done yet. Therefore, in this study synthesis of single layer MoS2 by using conventional chemical vapor deposition, as MoO3 and sulfur powder, we observe and discuss the synthesized crystal shape on the substrate, according to the distance of sulfur and MoO3. The synthesized nano-crystals were characterized by optical microscopy (OM), x-ray diffraction (XRD), raman spectroscopy. Fig. 1. shows the OM-image and raman spectra of synthesized MoS2, MoO2 crystals on S1 and S2 substrate, respectively. MoS2 crystals are synthesized on the S1 substrate close to the sulfur source, MoO2 crystals are synthesized on the S2 substrate. From these results, we were able to studies the mechanism of MoS2 synthesis. In the synthesis of MoS2, using a MoO3 and sulfur powder, the synthesis mechanism was shown as a schematic of the various experiments and in-depth understanding.

Therefore, we have demonstrated that the importance of MoO2 formation as the intermediate phase in MoS2 synthesis using MoO3 and sulfur powder. And then, the MoS2 synthesis mechanism was easier to understand through the schematic illustration.

2D-ThP4 Graphene Micro Wires Defined by Photolithography and Plasma Etching for Field Effect Transistors, *F.C. Rufino, A.M. Pascon,* University of Campinas, Brazil*; D.G. Larrude,* Mackenzie Presbyterian University, Brazil*; W.C. Mariano,* ***José Alexandre Diniz**,* University of Campinas, Brazil

With the need of the development of smaller devices, the search for materials with physical and chemical properties favorable to these advances has become a priority. However, Moore's Law is no longer verified [1], reinforcing research into new technologies, with a strong focus on 2D materials. The graphene, a 2D material, composed of sp2 hybrid carbon atoms, emerges as a strong candidate in nanotechnology applications due to its outstanding electronic properties, high electrical conductivity, mobility, flexibility, mechanical strength and transparency [2], making it the ideal material to replace the silicon in the traditional FETs.

We report the fabrication of transistors based on graphene channel (GraFETs), applying the photolithography and oxygen plasma etching processes to define the graphene channel region, creating ten micro wires, which are parallel connected, at the same device, as FinFET transistors based on silicon nanowires. Usually, the graphene channel region is not formed by the wires in parallel, but by square or rectangular shapes. Devices, with wires in parallel, can get an increase in drain-source current and the transconductance response, which can improve the sensitivity of sensors based on GraFETs. Thus, in this work is presented the fabrication of GraFETs with: i) High quality CVD (Chemical vapour deposition) monolayer graphene, which was transferred on the GraFETs; ii) The channel, with total width of 3.6 µm, was formed by ten micro wires in parallel, with each width of about 0.36 µm, (obtained by lithography and O_2 plasma etching).

The Raman spectroscopy was used to investigate the integrity of graphene structure on GraFETs during the fabrication. The Scanning Electron Microscopy (SEM) was used to show the channel formation with ten graphene wires and to measure the dimensions of these wires. The drain-source current versus drain-source voltage, the drain-source current versus gate voltage, and the transconductance versus gate voltage, were extracted to evaluate the electrical characterization of our GraFETs. The graphene used in the manufacture of the transistor was obtained through CVD, where the graphene is grown on a copper substrate by surface catalysis of the CH_4 and H_2 gases [3]. The growth process is done in a CVD chamber with a vacuum of 10^{-3} torr and a temperature of 1000 ºC, the transference of CVD monolayer graphene on the device region using wet transfer method and PMMA as a supporting layer [4].

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2D-ThP6 In-Operando AFM/STM and Transport Measurements of a Graphene Hall Bar Device, ***Johannes Schwenk,*** National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; S. Kim,* National Institute of Standards and Technology (NIST) / Department of Physics and Astronomy, Seoul National University, Seoul, Korea*; F. Ghahari,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; J. Berwanger,* Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany*; W.G. Cullen, S.R. Blankenship,* National Institute of Standards and Technology (NIST)*; Y. Kuk,* Department of Physics and Astronomy, Seoul National University, Seoul, Korea*; F.J. Giessibl,* Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany*; N.B. Zhitenev, J.A. Stroscio,* National Institute of Standards and Technology (NIST)

We present initial studies of a backgated graphene Hall bar device using simultaneous measurements of atomic force microscopy (AFM), scanning tunneling microscopy (STM) and electronic transport. Laterally resolved spectroscopy with high energy resolution is used for the investigation of exotic ground states and edge channels within the two-dimensional graphene electron system, which enables us to explore links between the local microscopic behavior of the device and its mesoscopic transport properties.

A recently constructed microscope uses a self-sensing quartz sensor (qPlus) and operates in an ultra-high vacuum (UHV) environment inside a dilution refrigerator (DR) with a base temperature of 10 mK and magnetic fields up to 15 T [1]. Radio frequency (RF) filtering of all signal lines entering the UHV chamber and improved home built RF powder filters at the 10 mK stage were implemented to produce an improved energy resolution in tunneling spectroscopy. Low noise preamplifiers for the sensor deflection [2] and the STM current signal [3] were implemented at the 4 K stage within the DR. This allows for reduced Johnson noise of the amplifier feedback resistors and a relatively short distance (1.2 m) between amplifier and the STM/AFM module where the sensor is operating. In this poster we describe aspects of the instrumentation and initial measurements of the graphene Hall bar device.

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2D Materials Focus Topic
Room 201B - Session 2D+EM+MN+NS-FrM

Nanostructures including Heterostructures and Patterning of 2D Materials

Moderator: Xiang Zhang, University of California, Berkeley

8:20am **2D+EM+MN+NS-FrM1 Interfacial Strength and Surface Damage Characteristics of Two-dimensional h-BN, MoS_2 and Graphene**, ***Frank DelRio,*** National Institute of Standards and Technology*; B.C. Tran Khac, K.H. Chung,* University of Ulsan, South Korea

Two-dimensional (2D) materials such as single- and multi-layer hexagonal boron nitride (h-BN), molybdenum disulfide (MoS_2), and graphene have attracted intensive interest due to their remarkable material properties. In this study, the film-to-substrate interfacial strengths and surface damage characteristics of atomically-thin h-BN, MoS_2 and graphene were systematically investigated via atomic force microscopy (AFM)-based progressive-force and constant-force scratch tests and Raman spectroscopy. The film-to-substrate interfacial strengths of these atomically-thin films were assessed based on their critical forces (*i.e.*, normal force where the film was delaminated from the substrate) as determined from progressive-force scratch tests. The evolution of surface damage with respect to normal force was further investigated using constant-force tests. The results suggested three different steps in the evolution of surface damage. At relatively low normal force, no significant change in topography and friction force was observed, which points to elastic deformation in the scratched area. As normal force increased, the formation of defects in the film and plastic deformation in the substrate were noted. At this stage, although the films have not yet failed, their topography, friction force, crystalline quality, and mechanical strengths were affected, which notably degraded their tribological performance. At normal forces above the critical force, delamination of the film from the substrate occurred. The compressive strain-induced buckling in front of the AFM tip was the primary source of mechanical instability. As the compressive strain increased, the atomic bonds were compressed, and eventually ruptured. As the number of layers increased, the tribological performance of h-BN, MoS_2, and graphene were found to significantly improve due to an increase in the interfacial strengths and a decrease in the surface damage and friction force. In all, the findings on the distinctive surface damage characteristics and general failure mechanisms are useful for the design of reliable nanoscale protective and solid-lubricant coating layers based on these 2D materials.

9:00am **2D+EM+MN+NS-FrM3 Sequential Edge-epitaxy: Towards Two-dimensional Multi-junctions Heterostructures and Superlattices**, ***Humberto Rodriguez Gutierrez,*** University of South Florida **INVITED**

Atomically thin layers are known as two-dimensional (2D) materials and have attracted a growing attention due to their great potential as building blocks for a future generation of low-power and flexible 2D optoelectronic devices. Similar to the well-established 3D electronics, the development of functional 2D devices will depend on our ability to fabricate heterostructures and junctions where the optical and electronic properties of different compounds are brought together to create new functionalities. Vertical heterostructures can be produced by selective van der Waals stacking of different monolayers with distinct chemical composition. However, in-plane lateral heterostructures, where different materials are combined within a single 2D layer, have proven to be more challenging. During the formation of the hetero-junction, it is important to minimize the incorporation of undesired impurities and the formation of crystal defects at the junction that will impact the functionality of the 2D device. When fabricating periodic structures it is equally important to develop the ability to control the domain size of each material. In this talk, we will review different techniques that have been used to create 2D lateral heterostructures of transition metal dichalcogenide compounds. Emphasis will be made in our recently reported one-pot synthesis approach, using a single heterogeneous solid source, for the continuous fabrication of lateral multi-junction heterostructures of TMD monolayers. In this method, the heterojunctions are sequentially created by only changing the composition of the reactive gas environment in the presence of water vapor. This allows to selectively control the water-induced oxidation and volatilization of each transition metal precursors, as well as its nucleation on the substrate, leading to sequential edge-epitaxy of distinct TMDs. This simple method have proven to be effective for continuous growth of TMD-based multi-junction lateral heterostructures, including selenides, sulfides and ternary alloys. Basic devices with field effect transistor configuration were fabricated to study the electrical behavior of these heterojunctions, their diode-like response, photo-response as a function of laser power as well as photovoltaic behavior of the heterojunctions will be discussed.

9:40am **2D+EM+MN+NS-FrM5 Interpretation of π-band Replicas Observed for Mono- and Multi-layer Graphene Grown on 4H SiC(0001)**, *T.B. Balasubramanian, M. Leandersson, J. Adell, C. Polley,* Lund University, Sweden*; **Leif Johansson**, R. Yakimova, C. Jacobi,* Linkoping University, Sweden

Graphene has made a major impact on physics due to its large variety of properties. The peculiar band structure of free standing graphene, showing linear dispersion and a Dirac point at the Fermi energy, makes it attractive for various applications. Large-scale epitaxial films have been grown on Si-terminated SiC substrates. However, the electronic structure is influenced when the graphene is laid upon a substrate whose lattice symmetry does not match that of graphene [1,2]. Six replicas oriented around each Dirac cone were observed already in the first ARPES experiments [1] of graphene grown on SiC(0001), and later reported [2] to have around 40 times lower intensity than a main Dirac cone. They were found to have the same relative separation and orientation as the rosette spots observed around the 0;th and 1x1 SiC and Graphene spots in the low energy electron diffraction (LEED) pattern and were explained [2] to have similar origin, i.e. to originate from photoelectron diffraction.

In two later ARPES investigations [3,4] additional weaker replicas were reported to exist along the Γ-K direction in the Brillouin zone of Graphene. One of them showed the existence [3] only for 1 ML but not 2 ML samples while the other reported [4] the existence in both 1 ML and 3 ML graphene samples. The origin of these replicas were in both cases attributed to a modulation of the ionic potential in the graphene layer/layers induced by the charge modulation of the carbon layer at the interface, i.e. the carbon buffer layer. Thus to an initial state effect instead of the earlier proposed final state effect. In both those experiments un-polarized HeI radiation was utilized, so the symmetry of the π-band replicas was not determined. We therefore investigated monolayer and multilayer graphene samples using linearly polarized synchrotron radiation, which allowed us to exploit the so called dark corridor [5] to directly determine the symmetry of the replica cones. Our ARPES data therefore clearly show the origin of these additional replicas observed using He-I radiation and moreover reveal the existence of some weaker replicas not earlier reported. An interpretation of our ARPES data in terms of final state photoelectron diffraction effects is shown to account for the location and symmetry of the π-band replicas observed.

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10:00am **2D+EM+MN+NS-FrM6 Effect of SiC(0001) Substrate Morphology and Termination on Multilayer Hexagonal Boron Nitride Epitaxy by Plasma-Enhanced CBE**, ***Daniel J. Pennachio,*** *N.S. Wilson, E.C. Young, A.P. McFadden, T.L. Brown-Heft,* University of California at Santa Barbara*; K.M. Daniels, R.L. Myers-Ward, D.K. Gaskill, C.R. Eddy, Jr.,* U.S. Naval Research Laboratory*; C.J. Palmstrøm,* University of California at Santa Barbara

Despite the prevalent use of hexagonal boron nitride (hBN) in 2D devices as a gate dielectric, tunnel barrier, or substrate, the quality of hBN thin films are typically lacking relative to flakes exfoliated from bulk crystals. To address the challenges of hBN epitaxy, this work studies the growth of hBN on single-crystal epitaxial graphene on SiC(0001) via plasma-enhanced chemical beam epitaxy (PE-CBE). As PE-CBE is conducted in an ultra-high vacuum environment, hBN nucleation, composition, and morphology were able to be examined using a combination of *in-situ, in-vacuo,* and *ex-situ* characterization techniques to gain insight into the formation of high-quality hBN films and hBN/graphene heterostructures.

It was found that utilization of high growth temperature (>1400°C) and nitrogen plasma flux (5×10^{-6} Torr background pressure) resulted in improved multilayer hBN film morphology over lower temperature (1300°C) depositions and CBE growths without nitrogen plasma flux. PE-CBE also produced more stoichiometric films than CBE without plasma at temperatures above 1400°C, as determined by *in-vacuo* X-ray photoelectron spectroscopy (XPS). *In-situ* reflection high energy electron diffraction (RHEED) showed streaky diffraction patterns persisting throughout several nanometers of PE-CBE hBN growth, indicative of a

smooth, epitaxial film. Crystallinity and epitaxial arrangement of hBN nuclei were examined by *in-vacuo* and *ex-situ* scanning probe microscopy (SPM). Scanning probe spectroscopy provided information on the electrical properties of the hBN films relative to bulk values.

The epitaxial alignment of the hBN/graphene/SiC(0001) heterostructure was studied by RHEED and by comparing nuclei edge alignment, as measured with SPM or scanning electron microscopy, to the substrate lattice orientation. It was found that the rotational alignment of the hBN nuclei depended on the substrate surface morphology. Nuclei on the (6√3×6√3)R30° SiC surface reconstruction, a graphene-like buffer layer, aligned directly to the buffer layer, while hBN nuclei on 4° off-cut epitaxial graphene substrates showed preferential alignment to substrate macrosteps rather than the graphene lattice. These ~25nm high macrosteps were then examined by cross-sectional transmission electron microscopy (TEM), which showed that the epitaxial graphene and hBN conformally blanketed the macrostep facets despite the macrostep's effect on nuclei orientation. The macrostep-directed nucleation outlined in this work provides a potential route to controlling the hBN/graphene rotational alignment during van der Waals epitaxy, an important variable for modulating electronic properties in this 2D system.

10:20am **2D+EM+MN+NS-FrM7 Nanoelectromechanical Drumhead Resonators from 2D Material Bimorphs**, ***Sun Phil Kim***, *J. Yu, E. Ertekin, A.M. van der Zande,* University of Illinois at Urbana-Champaign

Atomic membranes of monolayer 2D materials represent the ultimate limit in size of nanoelectromechanical systems. Yet, new properties and new functionality emerge by looking at the interface between layers in heterostructures of 2D materials. In this talk, we demonstrate the integration of 2D heterostructures as nanoelectromechanical systems and explore the competition between the mechanics of the ultrathin membrane and the incommensurate van der Waals interface. We fabricate electrically contacted, 5-6 µm circular drumheads of suspended heterostructure membranes of monolayer graphene on monolayer molybdenum disulfide (MoS_2), which we call a 2D bimorph. We characterize the mechanical resonance through electrostatic actuation and laser interferometry detection. The 2D bimorphs have resonance frequencies of 5-20 MHz and quality factors of 50-700, comparable to resonators from monolayer or few layer 2D materials. The frequencies and eigenmode shape of the higher harmonics display split degenerate modes showing that the 2D bimorphs behave as membranes with asymmetric tension. The devices display dynamic ranges of 44 dB, but there is a strong dependence of the dissipation on the drive. Under electrostatic frequency tuning, devices display small tuning of ~ 20% compared with graphene resonators > 100%. In addition, the tuning shows a recoverable kink that deviates from the tensioned membrane model for atomic membranes, and corresponds with a changing in stress of 0.014 N/m. One model that would account for this tuning behavior is the onset of interlayer slip in the heterostructure, allowing the tension in the membrane to relax. Using density functional theory simulations, we find that the change in stress at the kink is much larger than the energy barrier for interlayer slip of 0.0001 N/m in a 2D heterostructure, but smaller than the energy barrier for an aligned bilayer of 0.034 N/m, suggesting local pinning effect at ripples or folds in the heterostructure. Finally, we observe an asymmetry in tuning of the full width half max that does not exist in monolayer materials. These findings demonstrate a new class of NEMS from 2D heterostructures and unravel the complex interaction and impact of membrane morphology, and interlayer adhesion and slip on the mechanics of incommensurate van der Waals interfaces.

10:40am **2D+EM+MN+NS-FrM8 Atomically-precise Graphene Etch Masks for 3D Integrated Systems from 2D Material Heterostructures**, ***Jangyup Son***, University of Illinois at Urbana-Champaign*; A.M. van der Zande,* University of Illinois at Urbana Champaign

Atomically-precise fabrication methods are critical for the development of next-generation technologies in which electronic, photonic, and mechanical devices approach the atomic scale. In no area is this challenge more apparent than in nanoelectronics based on two-dimensional (2D) heterostructures, in which van der Waals (vdW) materials, such as graphene, hexagonal boron nitride (hBN), and transition metal dichalcogenides (TMDs), are integrated stacked to form functional electronic devices with nanometer thicknesses. A major challenge in the assembly of vdW heterostructure devices is the difficulty of patterning and individually connecting each molecular layer.

In this presentation, we demonstrate the use of graphene as a highly selective, atomically-thin etch mask and etch stop in van der Waals heterostructures. we also show the advantages of graphene etch masks (GEM) through advanced device demonstrations. We demonstrate that most inorganic 2D materials, such as hBN, TMDs, and black phosphorus (BP), are efficiently etched away by exposing those to XeF_2 gas at room temperature. In contrast, instead of getting etched, atomically-thin monolayer graphene is chemically functionalized (*i.e.* flurographene (FG)) under XeF_2 exposure due to the formation of sp^3 bonds by the addition of fluorine atoms onto the graphene surface. Based on this, we used exfoliated (and CVD) graphene layer as etch mask for patterning other 2D layers in micro (and macro) scale vdW heterostructures. We also demonstrate the use of this selective etching and GEM in mainly two different applications: 3D-integrated heterostructure devices with interlayer vias and suspended graphene mechanical resonators. First, we fabricate an electrical device having buried contacts in a 2D material heterostructure. Holes were etched through the top layer of hBN in an encapsulated BN-G-BN heterostructure to locally expose the buried graphene layer and contacts were fabricated by evaporating metal electrodes on the exposed graphene regions. The resulting encapsulated graphene device shows a low contact resistance of ~ 80 ohm·mm (n = -2×10^{12} cm^2) at room temperature, leading to high carrier mobility of ~ 140,000 $cm^2V^{-1}s^{-1}$, which is comparable to the electrical properties of state-of-the-art edge contacted graphene devices. Second, we fabricate a suspended graphene membrane by vapor phase etching of a BP thin film supporting graphene. We show that the graphene membrane behaves as a nanomechanical resonator with a frequency of 5.24 MHz and quality factor of ~255, comparable to graphene NEMS prepared on conventional substrates.

11:00am **2D+EM+MN+NS-FrM9 Insights into the O Atom Adsorption and O_2 Dissociation on Halogenated Graphene Surfaces**, ***Reynaldo Geronia***, University of the Philippines Diliman*; A.A.B. Padama,* University of the Philippines Los Baños, Philippines*; J.D. Ocon,* University of the Philippines Diliman, Philippines*; P.-Y. A. Chuang,* University of California, Merced

Oxygen reduction reaction (ORR) usually depends on precious metal-based catalysts like platinum and its alloys to facilitate its sluggish kinetics. The high cost of these materials however limits the employment of ORR-based technologies in commercial applications like fuel cells and metal-air batteries. Interestingly, recent works have demonstrated that doped metal-free carbon catalysts, such as graphene-based materials, can facilitate adsorption of ORR intermediate species [1]. This motivates us to investigate the interaction of oxygen atom and oxygen molecule on halogenated graphene systems.

In this work, we performed density functional theory (DFT) based calculations to investigate the stability of coplanar and non-coplanar halogen (X = F, Cl, Br, I) doped monovacant graphene systems. The stability of halogenated-graphene is strongly influenced by the size of halogen dopant as well as the geometry of the vacancy [2]. The calculated adsorption properties of atomic [3] and molecular oxygen on halogenated graphene systems, on the other hand, signifies the possibility of O_2 dissociation. We note that the dissociation of the molecule results to the distortion of the geometric structure of the substrate. This leads mostly to the formation of dangling and bridging C-O bonds along the edge of the graphene monovacancy which could have facilitated the dissociation of the molecule. Depending on the halogen, adsorption of oxygen can strengthen or weaken existing C-X bonds, due to differences between the abilities of oxygen and halogens to induce charge transfer and to participate in π bonding with carbon. These findings are expected to increase our understanding of novel graphene-based materials, which are currently being developed with the aim of reducing the use of noble metals as catalysts in fuel cells.

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