Friday Morning, November 11, 2016

2D Materials Focus Topic
Room 103B - Session 2D+NS-FrM

2D Materials: Device Physics and Applications

Moderator: Miguel M. Ugeda, CIC nanoGUNE, Spain

8:20am **2D+NS-FrM1 Direct Writing of 2D Flexible Electronic Devices via Illumination-based Techniques**, *M.E. McConney, N.R. Glavin, A.T. Juhl,* Air Force Research Laboratory; *J.E. Bultman, J.J. Hu,* University of Dayton Research Institute/Air Force Research Laboratory; *M.F. Durstock,* Air Force Research Laboratory; *A.A. Voevodin,* University of North Texas; ***Christopher Muratore,*** University of Dayton

Ultra-thin two-dimensional (2D) semiconducting materials possess a combination of large, tunable electronic bandgaps, optical transparency, and mechanical flexibility, and will likely revolutionize electronic devices such as wearable sensors and flexible displays. A primary step in the development of such devices with integrated 2D materials is the development of scalable, transfer-free synthesis over large areas at low temperatures. Electrically insulating amorphous transition metal dichalcogenide (TMD) films can be deposited via physical vapor deposition on large area flexible substrates at room temperature, and crystallized with subsequent illumination with light. Focused laser light with a power density of ~1 kW $cm^2$is suitable for writing micron scale features in semiconducting transition metal dichalcogenides on polymer substrates. Broad band illumination from a xenon lamp can also be used over the large substrate areas (> 100 cm^2), or passed through a physical mask to print features only in desired locations. The semiconducting properties of 2D MoS_2 and WS_2 materials synthesized in this way have been characterized using conductive atomic force microscopy, and other techniques to observe the expected temperature dependence on electrical conductivity. Structure and composition of the materials can be controlled by altering the incident fluence as well as by controlling the ambient environment during illumination, as verified by Raman spectroscopy, X-ray photoelectron spectroscopy, cross-sectional and plan view transmission electron spectroscopy, and other techniques. Multiple layers of 2D materials can also be treated in this way. For example, both layers in a MoS_2/WS_2 heterostructure of 10 nm total thickness on a polymer (PDMS) substrate were crystallized upon laser illumination. Diverse 2D architectures and devices built from illumination-based crystallization techniques will be highlighted.

8:40am **2D+NS-FrM2 Resolving and Tuning Mechanical Anisotropy in Black Phosphorus Nanoelectromechanical Resonators**, ***Zenghui Wang***, *H. Jia, P.X.-L. Feng,* Case Western Reserve University

Black phosphorus (P) has emerged as a layered semiconductor with unique crystal structure featuring corrugated atomic layers and strong in-plane anisotropy in its physical properties. In particular, it is predicted to exhibit strong in-plane mechanical anisotropy, which shall lead to previously inaccessible dynamic responses in resonant 2D nanostructures [1], and new opportunities for studying carrier-lattice interaction in atomic layers. It is therefore of both practical and fundamental importance to systematically investigate the mechanical anisotropy in black P crystal and NEMS devices.

Enabled by the first demonstration of black P resonant nanostructures [2] with multimode responses, we show that the spatial mapping of the multimode resonance mode shapes [3] creates a new means for precise determination of black P crystal orientation (*i.e.*, the anisotropic zigzag and armchair axes) [4] . Further, the multimode technique enables simultaneous quantification of the anisotropic mechanical properties (*i.e.*, elastic moduli along both major crystal axes): combined with finite element method (FEM) modeling, we determine the Young's moduli of multilayer black P to be 116.1 GPa and 46.5 GPa in zigzag and armchair directions, respectively. In addition, we demonstrate that electrostatic gating induced straining can continuously tune the mechanical anisotropic effects on multimode resonances in black P electromechanical devices. Our results show that multimode resonant response manifests the unique mechanical anisotropy effect in black P nanodevices, and provides a new method for determine the material's crystal orientation and elastic properties *in situ*, independent from conventional optical, electrical, and nanoindentation calibration techniques.

[1] Wang, Z. & Feng, P. X.-L. Design of Black Phosphorus 2D Nanomechanical Resonators by Exploiting the Intrinsic Mechanical Anisotropy. *2D Materials* **2,** 021001 (2015).

[2] Wang, Z., Jia, H., Zheng, X.-Q., Yang, R., Wang, Z., Ye, G.J., Chen, X.H., Shan, J., & Feng, P. X.-L. Black Phosphorus Nanoelectromechanical Resonators Vibrating at Very High Frequencies. *Nanoscale.* **7**, 877 (2015).

[3] Wang, Z., Lee, J., & Feng, P. X.-L. Spatial Mapping of Multimode Brownian Motions in High Frequency Silicon Carbide (SiC) Microdisk Resonators. *Nature Communications* **5**, 5158 (2014).

[4] Wang, Z., Jia, H., Zheng, X.-Q., Yang, R., Ye, G.J., Chen, X.H., & Feng, P. X.-L. Resolving and Tuning Mechanical Anisotropy in Black Phosphorus via Nanomechanical Multimode Resonance Spectromicroscopy. *under review.* (2016).

9:00am **2D+NS-FrM3 2D Devices for Flexible and Topological Nanoelectronics**, ***Li Tao***, *W. Zhu, D. Akinwande,* The University of Texas at Austin **INVITED**

Two-dimensional (2D) buckled atomic sheets, such as silicene and phosphorene, yield collective properties of mechanical flexibility and tunable bandgap, which hold promise for advanced flexible and topological nanoelectronics. Silicene is the 2D silicon equivalent of graphene, and is predicted to offer a host of exotic electrical properties, such as quantum spin Hall effect, subjected to external fields. Despite great theoretical expectations on silicene, air-stability had prevented experimental device studies. Recently, our research progress debuts silicene transistors corroborating theoretically predicted ambipolar transport with Dirac band structure. Electrostatic characterization on non-optimized silicene transistors exhibited carrier mobility ~100 cm^2/V-s and 10× gate modulation in ambient condition. Without non-ideal limiting factors, e.g. phase boundary scattering and electron-phonon coupling, pristine free-standing silicene is predicted to offer intrinsic mobility ~1200 cm^2/V-s. Further optimization is on-going to shed light on the mobility upper bound achievable and aging evolution of silicene devices. It is likely with further experimental study that monolayer or multilayer silicene can be a platform for realizing advanced device concepts, e.g. topological bits, on flexible substrates. The unique allotropic affinity of silicene with crystalline bulk silicon suggests a more direct integration with ubiquitous semiconductor technology.

Phosphorene, few-layer black phosphorus (BP), is another promising candidate for flexible nanoelectronics. Phosphorene exhibits high carrier mobility (100 to 1000 cm^2/Vs) and tunable direct bandgap (0.3 to 2eV) even on plastic substrates, making it the most suitable contemporary 2D semiconductor that combines the merits of graphene and transitional metal dichalcogenides. We reported the first BP based flexible RF transistors with intrinsic f_T=20 GHz and f_{Max}=14.5 GHz, and such performance sustained under ex-situ bending test with tensile strain up to 1.5%. Raman spectroscopy analysis of few-layer BP under tensile strain up to 7% was carried out for the first time to reveal the strain effect on BP. Significant orientation dependence was observed while applying tensile strain along armchair (AC) and zigzag (ZZ) directions, exhibiting the trend of Raman peak shift well agreed with theoretical projections. This recent progress on silicene and phosphorene represent a renewed opportunity for future nanoscale flexible and topological electronics beyond what is available in graphene.

9:40am **2D+NS-FrM5 Optical Detectors Based on Bismuth Telluride Nanowire Arrays Capped by Graphene**, ***Tito Huber***, *T. Brower, O. Abana,* Howard University

Recently, research on graphene based photodetectors has drawn substantial attention. The gapless nature of graphene and low light absorption can cause low responsivity. The synergetic integration of graphene with other materials is a promising approach to overcome these shortcomings. There have been reports of broadband photodetectors based on heterostructructures of few-layer Bi(2)Te(3)/graphene devices that are very encouraging. Here we discuss a different approach, where single layer graphene caps the top of a bismuth telluride nanowire array

(where the wire axis are perpendicular to the graphene surface) . Partially, our motivation was to test the exceptional thermoelectric properties of the interface. The room-temperature thermoelectric efficiencies of bismuth telluride compounds are the highest reported for any material, and, therefore, Bi(2)Te(3) nanowires are interesting as building blocks of nanoscale thermoelectric devices, as in this case. Graphene strong photothermoelectric response is also very well known. We employed devices composed of bismuth telluride nanowire arrays which are capped with single layer graphene. Dense arrays of 200-nm nanowires have been prepared by a nonlithographic fabrication technique consisting of the pressure injection of an alumina template with molten Bi_2Te_3, a method that can be successfully employed with 100-μm thick templates of pore diameters in the range of 2 to 200 nm. Bismuth telluride is a semiconductor with a small gap. The nanowire arrays electronic properties including magnetotransport and thermopower were characterized in separate experiments. The single layer graphene layer was fabricated by transfer by Graphenea. Graphene on the device was characterized using Raman spectroscopy. We observed the D, G and 2D peaks and broadening indicating that graphene is nearly intact. We also observed the Raman peaks of bismuth telluride. The incident surface features very low optical reflectivity and enhanced light trapping. Light trapping causes strong light absorption at the interface, an effect that counteracts the weak absorption of graphene and has not been mentioned in the literature before. The unique attributes of the thermoelectric arrays are the combination of strong temporal and optical wavelength dependences of the photocurrent. Under infrared illumination, the signal can be completely described by thermoelectric effects considering cooling rates given by heat diffusion through the array. We will discuss that, in addition, under visible illumination we observe a photovoltaic response. This work was supported by the National Science Foundation through PRDM 1205608 and STC 1231319

10:00am **2D+NS-FrM6 Graphene Nanoelectromechanical Resonators with Eletrothermal Excitation and Tuning**, *F. Ye,* ***Jaesung Lee****, P.X.-L. Feng,* Case Western Reserve University

Graphene, a hallmark of two-dimensional (2D) materials, has been employed as an atomically thin building block for highly miniaturized nanoelectromechanical system (NEMS) and shown attractive potential for nanoscale actuators and sensors. Thanks to its exceptional elastic modulus (E_Y~1TPa), ultralow mass density (r~2200kg/m^3), and superior strain limits (e_{limit}~25%) [1], high performance and frequency tunable graphene resonators have been demonstrated using photothermal [2] and electrostatic actuation [3] schemes. In addition to excellent mechanical properties, graphene possesses high temperature stability [4] and negative thermal expansion coefficient [5], hence graphene resonators may inherently exhibit better performance under high temperature. In existing reports, graphene resonators are exposed in high temperature using annealing or Joule heating (*e.g,*, applying up to 1.8V from drain to source) only for thermal annealing [3], high temperature operation of graphene resonators has not been demonstrated yet.

In this work, we fabricate mono- and bi-layer (1L and 2L) graphene resonators and investigate their resonance characteristics at high temperature up to ~500 K using Joule heating. We conveniently use DC voltage to heat graphene resonators, and apply AC voltage to excite resonance motion. Then, we simultaneously measure temperature and resonance characteristic of graphene resonators using a home-built, integrated Raman spectroscopy and laser interferometry measurement system. We first test electrothermal frequency tuning and find that frequency of graphene resonators upshift from ~80MHz to ~86MHz as DC voltage increases from 0.5V to 2.5V. Unlike electrostatic force resonance tuning and excitation [3], we do not observe capacitive softening or loaded *Q* effects which may compromise performance of resonators. We then investigate mechanical nonlinearity of graphene resonators in high temperature by changing both DC and AC voltage. This study opens new capabilities for engineering tunable graphene NEMS resonators and oscillators for a number of emerging applications.

[1] C. Lee, *et al.*, *Science***321**, 385-388 (2008).

[2] J. S. Bunch, *et al.*, *Science.***315**, 490-493 (2007).

[3] C. Chen, *et al.*, *Nat. Nanotech.***4**, 861-867 (2009).

[4] K. Kim, *et al.*, *Phys. Status Solidi RRL***4** 302-304 (2010).

[5] M. Pozzo, *et al.*, *Phys. Rev.Lett.***106** 135501 (2011).

10:20am **2D+NS-FrM7 Pushing the Performance Limit of 2D Semiconductor Transistors**, ***Xiangfeng Duan****,* California Nanosystems Institute, University of California, Los Angeles **INVITED**

Two-dimensional semiconductors (2DSCs) such as MoS_2 have attracted intense interest as an alternative electronic material in the post-silicon era. However, the on-current density achieved in 2DSC transistors to date is considerably lower than that of silicon devices. It remains an open question whether 2DSC transistors can offer competitive performance. To achieve a high performance (high on-current) device requires (1) a pristine channel with high carrier mobility, (2) an optimized contact with low contact resistance and (3) a short channel length. The simultaneous optimization of these parameters is of considerable challenge for atomically thin 2DSCs since the typical low contact resistance approaches either degrade the electronic properties of the channel or are incompatible with the fabrication of short channel devices. Here I will first review different strategies that have been developed to optimize these factors, and discuss how we can combine these strategies together to achieve high performance 2DSC semiconductor transistors. In particular, we will discuss a unique approach towards high-performance MoS_2 transistors using a physically assembled nanowire as a lift-off mask for creating ultra-short channel devices with pristine MoS_2 channel and self-aligned low resistance metal/graphene hybrid contact. With the optimized contact in short channel devices, we demonstrate that a sub-100 nm MoS_2 transistor can deliver a record a high on-current density comparing well with that of silicon devices, demonstrating thte exciting potential of 2DSCs for future electronic applications.

11:00am **2D+NS-FrM9 Low Temperature Al_2O_3 ALD on 2D Semiconductors**, ***Il Jo Kwak****, J.H. Park, A.C. Kummel,* University of California at San Diego

2D semiconductors have attracted attention for future electronic devices due to their excellent electronic and optoelectronic properties. These devices require few nanometer thick and pin hole-free dielectric layers as gate insulators. However, due to the inert nature of 2D semiconductors such as graphene and Transition Metal Chalcogenides (TMDs), the dielectric layer selectively nucleates on defect sites or step edges. In the conventional atomic layer deposition (ALD) process on graphene or other 2D semiconductors, such non-uniform oxides result in large leakage currents in 2D semiconductor based device. Therefore, for successful integration into device, uniform and insulating gate oxides on 2D semiconductors should be prepared.

In this work, Al2O3 was directly deposited on HOPG and MoS2 surface by low temperature ALD with trimethylaluminum(TMA) and H2O or O3 without any seeding layer or surface treatments. Using short purge time between two precursor pulses at 50C, a CVD growth component was intentionally induced to provide more nucleation sites on the surface. The CVD growth component induces deposition of 1 nm Al2O3x particles on the surface which provide a uniform layer of nucleation centers. Before ALD, HOPG and MoS2 samples were cleaned by mechanical exfoliation method. For HOPG substrate, 50 cycles of ALD Al2O3 was deposited at 50C using 600ms of TMA and 50 ms of H2O pulse time with 500ms purge time between two pulses. In the case of MoS2, 300ms of O3 pulse was employed instead of H2O pulse. The same ALD recipes were performed on SiGe substrates in order to compared the quality of the oxide. After ALD process, MOSCAP devices were fabricated to measure the capacitance and leakage current of the oxide. Non-contact mode AFM was performed to check the topography of the oxide and the results showed that uniform and pin hole-free oxide layer was formed on the surface. The leakage current of the oxide on HOPG and MoS2 was as low as 10^{-5} A/cm^2 which was comparable to the oxide on SiGe substrates.

11:20am **2D+NS-FrM10 Atomic Layer Deposition of High-k Dielectrics on WSe_2 for High Performance Electronic Devices**, ***Pushpa Raj Pudasaini****, M.G. Stanford, A. Hoffman,* The University of Tennessee Knoxville*; T.Z. Ward,* Oak Ridge National Laboratory*; D.G. Mandrus, P.D. Rack,* The University of Tennessee Knoxville

The performance of electronic and optoelectronic devices based on two-dimensional (2D) transition metal dichalcogenides (TMDs), such as tungsten diselenide (WSe_2) is significantly affected by the quality of the various interfaces present in the device. Historically, the performance of bottom-gate SiO_2 2D TMDs field effect transistor (FET) devices has been greatly limited by the carrier scattering due to the oxide trapped charges, surface roughness, and surface optical phonons, among others. One approach to mitigate this issue is to explore alternatives to SiO_2 which ideally would involve high-κ dielectrics, in which Coulombic impurity scattering is confirmed to be strongly shielded by the dielectric screening.

However, depositing high quality high-k dielectric film onto the surfaces of TMDs is very challenging due to the chemical inertness of the TMD basal planes. Here, we present an aluminum oxide and hafnium oxide top-gate on WSe_2, deposited using atomic layer deposition (ALD) both with and without hydrogen/oxygen plasma treatments and titanium seed layers. The top gated WSe_2 FET devices are fabricated by employing ALD deposited high k-dielectrics, with promising device characteristics having large current on-off ratio (~10^8), small threshold voltage (~5V) and relatively large field effect mobility (~70 cm^2/V.s) at room temperature. A high performance logic invertor device is also demonstrated.

11:40am **2D+NS-FrM11 Layer-dependent Measurements of Electronic Band Alignment for Individual MoS_2 Flakes Supported on SiO_2 using Photoemission Electron Microscopy (PEEM) with Deep Ultraviolet Illumination**, ***Morgann Berg,*** Sandia National Laboratories*; K. Keyshar,* Rice University*; I. Bilgin, F. Liu,* Northeastern University, Los Alamos National Laboratory*; H. Yamaguchi,* Los Alamos National Laboratories*; R. Vajtai,* Rice University*; C. Chan,* Sandia National Laboratories*; G. Gupta,* Los Alamos National Laboratories*; S. Kar,* Northeastern University*; P. Ajayan,* Rice University*; T. Ohta,* Sandia National Laboratories*; A. Mohite,* Los Alamos National Laboratories

Tailoring band alignment layer-by-layer using heterojunctions of two-dimensional (2D) semiconductors is an attractive prospect for producing next-generation electronic and optoelectronic devices that are ultra-thin, flexible, and efficient. 2D layers of transition metal dichalcogenides (TMDs) in laboratory devices have already demonstrated properties favorable for electronic and optoelectronic applications. Despite these strides, a systematic understanding of how band alignment evolves from monolayer to multilayer for MoS_2, a model TMD system, is still missing owing to the lack of a suitable experimental approach. Quantitative determination of the electronic band alignment necessitates that measurements be performed in a controlled environment (such as vacuum) using a substrate that interacts minimally with the overlying TMDs (preferably insulating) to suppress the electronic influence of supporting substrates and prevent chemical modification of TMDs due to adsorbates (primarily water).

Here we report on the local band alignment of monolayer, bilayer, and tri-layer MoS_2 on a 285-nm-thick SiO_2 substrate, measured using a new approach to probe the occupied electronic states based on photoemission electron microscopy with deep ultraviolet excitation. The spatially-resolved, simultaneous measurements of the vacuum level and the valence band edge at the Brillouin zone center show that the addition of layers to monolayer MoS_2 increases the relative work function, and pushes the valence band edge toward the vacuum level. We also find n-type doping of few-layer MoS_2 and type-I band alignment across monolayer-to-bilayer and bilayer-to-trilayer lateral junctions. Our results differ from some earlier reports based on Kelvin probe and scanning photocurrent microscopies [Sci. Reports, 5, 10990 (2015), Nano Lett., 15, 2278 (2015)], and highlight the strong influence of environmental effects on the band alignment in MoS_2 homojunctions. We are now applying this exciting new metrology to systematically examine the ionization energies of a series of TMDs. The results will provide fundamental information necessary to assess the band alignments of TMD heterojunction devices, and to validate or refine existing theoretical predictions [APL, 103, 053513 (2013), J. Phys. Chem. C, 119, 13169 (2015)].

This work was performed at CINT (DE-AC04-94AL85000), and is supported by Sandia LDRD, US DOE EERE SunShot Initiative BRIDGE (DE-FOA-0000654 CPS25859), and Army Research Office MURI (W911NF-11-1-0362). SNL is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Co., for the US DOE NNSA (DE-AC04-94AL85000).

12:00pm **2D+NS-FrM12 Visualizing Light Scattering in Silicon Waveguides with few-layer Black Phosphorous Photodetectors**, ***Tianjiao Wang,*** *S. Hu,* Vanderbilt University*; B. Chamlagain, Z. Zhou,* Wayne State University*; S.M. Weiss, Y. Xu,* Vanderbilt University

We investigate the light scattering properties of a silicon nanobeam waveguide through wavelength- and polarization-dependent scanning photocurrent measurements of a black phosphorus (BP) photodetector on top of the silicon waveguide. The measured photocurrent responses exhibit similar patterns as the light intensity distribution calculated by finite-difference time-domain simulations, suggesting that the light scattering properties of the waveguide can be detected as photocurrent signals by the BP photodetector. Interestingly, no photocurrent signals are observed when the incident photon energy is below the bandgap of silicon, indicating that the photocurrent response generated in the BP photodetector is mainly attributed to the photo-excited electron-hole pairs in the silicon waveguide which can be injected into the BP and dominate its photocurrent generation. Our experimental results suggest that two dimensional (2D) material based photodetectors can offer an effective approach to visualize the light scattering properties of photonic structures by photocurrent mapping, which not only opens up avenues for learning about light matter interaction of photonic structures but also provides a way of engineering future 2D material based optoelectronic devices with integrated photonic structures.

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