2D Materials Focus Topic
Room 103B - Session 2D+MI-ThM

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

Moderators: Paul Sheehan, US Naval Research Laboratory, Zhaohui Zhong, University of Michigan, Ann Arbor

8:00am **2D+MI-ThM1 Mechanics and Fracture of 2D Materials with Defects and Grain Boundaries**, ***Zhao Qin***, *G.S. Jung,* Massachusetts Institute of Technology*; S. Wang,* University of Oxford, UK*; F.J. Martin-Martinez,* Massachusetts Institute of Technology*; J.H. Warner,* University of Oxford, UK*; M.J. Buehler,* Massachusetts Institute of Technology

Two dimensional materials including graphene, silicene, MoS2 and so forth represent ideal materials composed of a single layer of atoms organized in a lattice form. Their unique geometry and intriguing mechanical and thermal properties make them perfect candidates for nano scale engineering applications. The robustness of the materials, especially those with defects is important to prevent their catastrophic failure and contribute to their durability in usage. Here we combine both large-scale molecular dynamics simulations based on reactive force fields and experiments via transmission electron microscopy to investigate their fracture behavior under extreme mechanical loading conditions. We focus on how defects and grain boundaries in 2D materials affect the critical conditions and the dynamics process of their fracture. Our results reveal that certain forms of atomic defects and grain boundaries are beneficial to enhance the mechanical strength of 2D materials that are subjected to cracks. For example, we find that poly-crystalline graphene under fracture releases up to 50% more energy than the pristine graphene. We find that grain boundaries increase the critical energy release rate to fracture by reducing stress concentration and making branches near the crack tip. We find atomic defects can cause crack deflections during crack propagation, effectively extending the crack length during propagation and thus increase the energy dissipation. Together, these molecular irregularities taking place at the atomic scale level can significantly affect the lattice characteristics of the 2D materials at larger scale levels and thereafter enhance their fracture toughness, making its crack propagation different from pristine ones, and such a mechanism explains the reduced crack propagation speed by adding vacancies as what is seen in experiments.

8:20am **2D+MI-ThM2 Effects of Non-local Screening and Effective Mass Anisotropy on Excitons in 2D Materials**, *I.I. Oleynik,* ***Joseph Gonzales***, University of South Florida

The optical excitations in semiconductors are substantially influenced by electron-hole interactions resulting in formation of excitons. Although the exciton binding energies in the bulk are much smaller that the fundamental band gaps, the excitonic effects in 2D materials are significantly amplified due to combined effect of quantum confinement and non-local screening of electron-hole interactions in two dimensions. An effective mass theory of 2D excitons, which takes into account the combined effect of the anisotropy and non-local 2D screening, is used to systematically investigate the variation of monolayer exciton binding energies E_x across a representative set of layered chalcogenides, both isotropic, such as $MoTe_2$, $MoSe_2$, WSe2, and WS_2, and anisotropic including phosphorene, TiS_3, ReS_2, and $SnSe_2$. The markedly different values of E_x are correlated with corresponding variations in atomic polarizabilities of constituent atoms.

8:40am **2D+MI-ThM3 2D Materials: A New Platform for Strong Light-Matter Interactions**, ***Ajit Srivastava***, Emory University **INVITED**

A recent addition to low-dimensional materials are monolayer transition metal dichalcogenides (TMDs), such as WSe_2, with an atomically thin, honeycomb lattice and optical band gaps. In addition to spin, charge carriers in TMDs exhibit a “valley” degree of freedom which can be optically addressed using circularly polarized light, opening up exciting possibilities for “valleytronics". Another curious aspect of TMDs lies in the non-trivial geometry of their band structure which gives rise to equal but opposite Berry curvature, an effective magnetic field in the momentum space. Owing to unusually strong Coulomb interactions in truly 2D limit, optical spectra of monolayer TMDs is dominated by tightly bound excitons which are expected to strongly couple to light and form stable polaritons - half light, half matter excitations.

In this talk, I will begin by presenting our recent results on valley Zeeman effect, where in analogy to spins, valleys shift in energy with magnetic field. Next, I will discuss our theoretical results on how the non-trivial geometry of Bloch bands modifies the excitonic fine structure of TMDs resulting in an orbital Zeeman effect in reciprocal space and a Lamb-like shift of levels. Finally, I will present our recent results on the observation of microcavity polaritons confirming the strong light-matter interactions in these materials. The presence of valley degree of freedom, non-trivial geometry of bands, and the possibility of introducing non-linearities in form of quantum emitters makes polaritons in TMDs particularly appealing for studying correlated many-body physics and topological states of matter.

9:20am **2D+MI-ThM5 Electronic Transport and Localization in Nitrogen-Doped Graphene Devices Using Hyperthermal Ion Implantation**, ***Adam Friedman***, *C.D. Cress,* Naval Research Laboratory*; S.W. Schmucker,* National Research Council postdoc working at Naval Research Laboratory*; J.T. Robinson, O.M.J. van 't Erve,* Naval Research Laboratory

Chemical alteration of graphene facilitates doping and may add a usable transport gap. For most published studies, atomic species (e.g., fluorine or hydrogen) are chemically bonded to the surface out-of-plane, breaking the sp^2 symmetry and replacing it with an sp^3 bond. These methods produce functionalized graphene, rather than substitutionally-doped graphene, where the former is typically only chemically stable for days (e.g., fluorine) or weeks (e.g., hydrogen) or less, depending on environmental conditions. Hyperthermal ion implantation offers a controllable method of producing high-quality substitutionally doped graphene with nitrogen, an n-type dopant that has great potential for graphene electronics and spintronics applications where high carrier concentration, uniform doping, and minimal vacancy defect concentration is desired [1]. Here we examine the transport properties of monolayer graphene sheets as a function of implantation beam energy and dose. We observe a transition from weak (metal) to strong (insulator) localization that varies as a function of carrier concentration, and we find that the transition is suppressed near the Dirac point for higher amounts of nitrogen [2]. For nominally equivalent doses, increased N ion energy results magnetoresistance magnitude increases, reaching a value as approximately -5.5% at 5,000 Oe, which we discuss in the context of dopant concentration and defect formation. We use a model for the temperature dependence of the conductivity that takes into account both temperature activation, due to the formation of a transport gap, and Mott variable-range hopping, due to the formation of defects, to further study the electronic properties of the doped films as a function of dose and N ion energy. We find that the temperature activation component dominates the behavior, further indicating that the implanted nitrogen, rather than defects, is responsible the observed result.

[1] C.D. Cress, et al. ACS Nano 10, 3714 (2016).

[2] A.L. Friedman, et al. Phys. Rev. B, 93 161409(R) (2016).

9:40am **2D+MI-ThM6 Metal Contacts to Transition Metal Dichalcogenide Films: Understanding and Avoiding the Formation of a Schottky-like Barrier**, *M. Gomez, J. Martinez, M. Valentin, E. Preciado, V. Klee, C. Merida,* ***Ludwig Bartels***, University of California - Riverside

We utilize a combination of X-ray photoelectron spectroscopy, transport measurements and optical as well as acoustic excitation to study the impact of the formation of metal contacts to transition metal dichalcogenide films on the electronic structure of the films. Photoelectron spectroscopy permits us to follow the formation of a Schottky-like barriers with increasing metal film thickness on the Angstrom scale. We utilize core level spectroscopy to indicate the evolution of the MoS_2 valence band during metal deposition. Our findings indicate that single layer MoS_2 films adopt the character of the metal (Fermi-level pinning) resulting in a Fermi-level position in the MoS_2 semiconducting gap that is – depending on the metal work function –indicative of a *p*-type semiconductor, even though the native carriers in an MoS_2 film are electrons. As a consequence, metal-TMD-metal junctions may best be understood as *p-n-p* junctions. Numerous ancillary measurements support this hypothesis.

11:00am **2D+MI-ThM10 Multilayer Graphene Suspension Over Millimeter Size Openings and Mechanical Testing**, ***Joseph Rowley***, *R.F. Davis, R.R. Vanfleet,* Brigham Young University*; J. Abbott,* Moxtek, Inc.

Because of it's high ultimate tensile strength, a single atomic layer of graphene has been able to suspend micron size holes reliably. However, to extend into regimes where devices have dimensions measured in millimeters, a single layer of graphene is insufficient. Films made from a few layers of graphene, although not as strong as pristine single layer graphene, have been shown to still retain a high level of strength. Using chemical vapor deposition on a nickel catalyst, we have fabricated many layer graphene films and suspended these membranes over millimeter size holes. Mechanical properties were measured on suspended films using a custom bulge test instrument.

11:20am **2D+MI-ThM11 Modeling Excitons in Transition-Metal Dichalcogenides**, *F. Tseng,* NRC Research Associate*; E. Simsek,* George Washington University*; **Daniel Gunlycke**,* Naval Research Laboratory

Using a triangular lattice exciton (3ALE) model, we explore exciton states in semiconducting monolayer transition-metal dichalcogenides. We show that the hydrogen model for excitons breaks down due to lattice effects and that the excitons are neither Wannier nor Frenkel excitons and instead span an intermediate size regime. The model is formulated on sparse form in direct space, leading to a computationally efficient N log(N) scaling and the ability to calculate over lattice grids with tens of thousands of sites, more than sufficient to converge exciton states in this intermediate exciton regime. In this presentation, we will also discuss the Coulomb potential generated from a dielectric substrate and how the exciton binding energies could be tuned by the thickness and permittivity of an oxide layer.

11:40am **2D+MI-ThM12 Characterization of Collective Ground States in Single-layer $NbSe_2$, *Miguel M. Ugeda*,** CIC nanoGUNE, Spain*; A.J. Bradley,* University of California at Berkeley*; Y. Zhang,* Advanced Light Source, Lawrence Berkeley National Laboratory*; S. Onishi, W. Ruan, Y. Chen, C. Ojeda-Aristizabal,* University of California at Berkeley*; H. Ryu,* Advanced Light Source, Lawrence Berkeley National Laboratory*; M.T. Edmonds, H.Z. Tsai, A. Riss,* University of California at Berkeley*; S.K. Mo,* Advanced Light Source, Lawrence Berkeley National Laboratory*; D. Lee, A. Zettl,* University of California at Berkeley*; Z. Hussain,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Z.X. Shen,* Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory*; M.F. Crommie,* University of California at Berkeley **INVITED**

Layered transition metal dichalcogenides (TMDs) are ideal systems for exploring the effects of dimensionality on correlated electronic phases such as charge density wave (CDW) order and superconductivity. In bulk $NbSe_2$ a CDW sets in at T_{CDW} = 33 K and superconductivity sets in at T_c = 7.2 K. Below T_c these electronic states coexist but their microscopic formation mechanisms remain controversial. In this tal I will present the electronic characterization study of a single 2D layer of $NbSe_2$ by means of low temperature scanning tunneling microscopy/spectroscopy (STM/STS), angle-resolved photoemission spectroscopy (ARPES), and electrical transport measurements (1). I will show that 3x3 CDW order in $NbSe_2$ remains intact in 2D. Superconductivity also still remains in the 2D limit, but its onset temperature is depressed to 1.9 K. Our STS measurements at 5 K reveal a CDW gap of Δ = 4 meV at the Fermi energy, which is accessible via STS due to the removal of bands crossing the Fermi level for a single layer. Our observations are consistent with the simplified (compared to bulk) electronic structure of single-layer $NbSe_2$, thus providing insight into CDW formation and superconductivity in this model strongly-correlated system. Furthermore I will show that CDW order is also present in 2D semiconducting TMDs around 1D mirror twin boundaries (2).

(1) M. M. Ugeda, et al., Nature Physics 12, 92 (2016).

(2) S. Barja, et al., Nature Physics, in press (2016).

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