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-TuM-1 Effect of Lattice Stacking Orientation and Local Thickness Variation on the Mechanical Behavior of Few Layer Graphene Oxide**, ***Teng Cui***, *S Mukherjee, C Cao, P Sudeep, J Tam,* University of Toronto, Canada*; P Ajayan,* Rice University*; C 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-TuM-2 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-TuM-3 Mechanical Properties of Many-layer CVD Graphene**, ***Kyle Larsen***, *S Lehnardt, J Rowley, B Anderson, R Vanfleet, R 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).

9:00am **2D+EM+MI+NS-TuM-4 Electronic Structure and Magneto-transport Properties of Nanostructured Graphene on SiC(001)**, ***Victor Aristov***, DESY Hamburg, Germany*; H Wu,* BIT, Beijing, China*; O Molodtsova,* DESY Hamburg, Germany*; A Chaika,* ISSP RAS, Russia

Graphene shows unbelievable properties that are of worth both for basic investigations and technology. The aptitude to open gap and to get graphene magnetic are principal challenges in the fields of up-to-date applications. Nanostructured graphene with an enormous amount of nano-domain boundaries and ripples becomes to be the most promising material for graphene-based electronic and spintronic applications, since nano-domain edges can completely reflect electrons over a great range of energies [1] and hold spin-polarized electronic states [2, 3]. Electrical measurements conducted at low temperatures on the vicinal SiC(001) samples demonstrate the opening of a transport gap in the nanostructured trilayer graphene up to 1.3 eV [4], which is induced by self-aligned periodic nanoboundaries . The transport gap opening produces high current on-off ratio of 10^4 [4, 5]. The magneto-resistance measurements disclose an exceptional big positive magneto-resistance in parallel magnetic field with strong temperature dependence [6]. It has been shown that graphene layer rippling near domain boundaries lead to one-dimensional conductivity (along the domain boundaries) at low temperatures and to accumulation of electrons with a particular spin direction at the boundaries. Moreover, nanodomain boundaries with ripples have the potential to work as a spin-filter and can result in a positive magnetoresistance at low temperature.

This work was supported by Beijing Institute of Technology Research Fund Program for Young Scholars, Science Foundation Ireland (SFI) (No. 12/IA/1264), Russian Foundation for Basic Research (Grant Nos. 17-02-01139, 17-02-01291), Marie Curie IIF grant within the 7th EC Framework Program.

1. O.V. Yazev and S.G. Louie, *Nature Mater*., **9**, 806 (2010).

2. P. Ruffieux et al.*,Nature,***531**, 489 (2016).

3. K. Nakada *et al.,Phys. Rev.,***B 54**, 17954 (1996).

4. H.-C. Wu, A.N. Chaika, et al., *ACS Nano,***9**, 8967 (2015).

5. A.N. Chaika, V.Yu. Aristov, O.V. Molodtsova, *Prog Mater Sci*., **89**, 1 (2017).

6. H.-C. Wu, A.N. Chaika, et al., *Nature Commun*., **8**, 14453 (2017).

9:20am **2D+EM+MI+NS-TuM-5 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-TuM-10 Onset of Buckling Folding and Slipping Instabilities in 2D Materials under Compressive Strain**, ***Jaehyung Yu***, *E Ertekin, A 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-TuM-11 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.

[i] Weinreich, G., Acoustodynamic effects in semiconductors. Phys. Rev. **104**, 321 (1956); http://dx.doi.org/10.1103/PhysRev.104.321

[ii] Hoskins, M. J.; Morkoç, H.; and Hunsinger, B. J., Charge transport by surface acoustic waves in GaAs. Appl. Phys. Lett. **41**, 332 (1982); https://doi.org/10.1063/1.93526

[iii] Miseikis, V.; Cunningham, J. E.; Saeed, K.; O'Rorke, R.; and Davies, A. G., Acoustically induced current flow in graphene. Appl. Phys. Lett. **100**, 133105 (2012); https://doi.org/10.1063/1.3697403

11:40am **2D+EM+MI+NS-TuM-12 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.

References: [1] V. Dorgan, M.-H. Bae, E. Pop, *Appl. Phys. Lett.* 97, 082112 (2010). **[2]** M. Yamoah, et al., *ACS Nano* 11, 9914 (2017). **[3]** M.-H. Bae et al., *Nature Comm.* 4, 1734 (2013). **[4]** S. Islam, et al., *IEEE Electron Device Lett*. 34, 166 (2013). **[5]** A. Behnam et al., *Appl. Phys. Letters*. 107, 123508 (2015). **[6]** N. Wang et al., *IEEE VLSI Tech. Symp*., Jun 2016, Honolulu HI. **[7]** K. Smithe et al., *ACS Nano* 11, 8456 (2017). **[8]** M. Mleczko et al., *ACS Nano* 10, 7507 (2016). **[9]** M. Mleczko, E. Pop, et al., *Science Adv.* 3, e1700481 (2017). **[10]** C. English et al., *Nano Lett*. 16, 3824 (2016). **[11]** C. English et al., *IEEE Intl. Electron Devices Meeting (IEDM)*, Dec 2016. **[12]** E. Yalon, E. Pop, et al., *Nano Lett.* 17, 3429 (2017). **[13]** A. Sood, E. Pop et al. *in press* (2018).

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