

Monday Afternoon, October 30, 2017

2D Materials Focus Topic

Room 15 - Session 2D+MI-MoA

Novel 2D Materials

Moderator: Kathleen McCreary, Naval Research Laboratory

2:00pm 2D+MI-MoA-2 Computational Characterization of 2D Perovskite Oxides Nanosheets, Yanfu Lu, S Sinnott, Pennsylvania State University

The metal oxides known as perovskites are well-known for a variety of useful properties, including piezoelectricity, ferroelectricity, and magnetism. The bulk form of these materials has been well-studied over the last few years with computational materials science methods to better understand their structure-property relationships. More recently, two-dimensional (2D) materials “beyond graphene” have attracted substantial attention because of the potential for electron confinement and engineering of the electronic structure. According to V. Gopalan & R. Engel-Herbert (*Nat. Mater.*, 2016), there are 389 theoretical predicted perovskite bulk structures, ABO_3 , where over half of them have been synthesized. When the same structure is synthesized in 2D form, the stoichiometry becomes $A_nB_{n-1}O_{3n+1}$. To identify perovskite oxides that may be produced as free-standing nanosheets, different thickness and different crystal orientation respect to the normal surface will be considered. When density functional theory (DFT) calculations are performing to each possibility, the accurate formation energy, lattice parameter, ionic polarization, and electronic bandstructure will be obtained to reveal the new ferroelectric, magnetic, and other properties associated with the formation of 2D materials from normally three-dimensional perovskite materials. The work performed here will consist of high-throughput first principles calculations. The results will be added to a searchable on-line database of 2D materials and freely disseminated to the community.

2:20pm 2D+MI-MoA-3 Electronic and Optoelectronic Physics in the van der Waals Heterojunctions, Philip Kim, Harvard University INVITED

Recent advances of van der Waals (vdW) materials and their heterostructures provide a new opportunity to realize atomically sharp interfaces in the ultimate quantum limit. We demonstrate the enhanced electronic optoelectronic performances in the vdW heterostructures, suggesting that these a few atom thick interfaces may provide a fundamental platform to realize novel physical phenomena, such as hydrodynamic charge flows, cross-Andreev reflection across the quantum Hall edges states, and interlayer exciton formation and manipulations.

3:00pm 2D+MI-MoA-5 Discovery of over 1000 New Two-dimensional Materials, 487 One-dimensional Molecular Wires and 98 Naturally Occurring Heterostructures, Gowoon Cheon, K Duerloo, A Sendek, C Porter, Y Chen, E Reed, Stanford University

Layered materials held together by weak interactions including van der Waals forces, such as graphite, have attracted interest for both technological applications and fundamental physics. Only a few dozen two-dimensional van der Waals solids have been subject to considerable research focus, although there likely to be many more and which could have superior properties. In this work, we identify 1173 two-dimensional layered materials and 487 materials that consist of weakly bonded one-dimensional molecular chains out of 58097 inorganic materials in the Materials Project. This is an order of magnitude increase in the number of identified materials, with most materials not known as two- or one-dimensional materials. To achieve this, we developed a novel data mining algorithm that determines the dimensionality of weakly bonded components contained in bulk, 3D crystal structures based on atomic bond lengths. Data mining allows for screening of all materials in the database, including but not confined to materials belonging to known families of two- or one-dimensional materials. Moreover, we identify 98 weakly bonded heterostructures that exist as bulk materials, opening new possibilities for much-studied assembly of van der Waals heterostructures.

Data on the families of materials, band gaps and point groups for the materials identified in this work are presented. Point group and piezoelectricity in layered materials are also evaluated in single-layer forms. 325 of these materials are expected to have piezoelectric monolayers with a variety of forms of the piezoelectric tensor. This work significantly extends the scope of potential low-dimensional weakly bonded solids to be investigated.

4:00pm 2D+MI-MoA-8 Anisotropic 2D Palladium Diselenide with High Mobility for Air-stable Electronics, Akinola Oyedele, University of Tennessee; L Liang, A Puzetzy, S Yang, A Strasser, C Rouleau, B Sumpter, D Geohagan, Oak Ridge National Laboratory; K Xiao, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Two-dimensional crystals are emerging materials for the realization of nanoelectronic devices including transistors, photodetectors, and chemical sensors. These ultra-thin electronics require candidate systems with high carrier mobility, sizeable and tunable bandgaps, and air stability, which are important for high-speed, durable applications. We present a new candidate, palladium diselenide ($PdSe_2$), with a similar puckered structure to black phosphorus, into the growing family of 2D materials. $PdSe_2$ exhibits a strong layer-dependent bandgap variation from ~ 0.2 eV (bulk) to ~ 1.3 eV (monolayer), and an electron mobility as high as ~ 330 $cm^2V^{-1}s^{-1}$ for few-layer systems. Due to their low-symmetry, $PdSe_2$ exhibits very interesting anisotropic behavior and the strong interlayer interaction is revealed from the large thickness-dependent Raman peak shifts, agreeing with first-principles Raman simulations. Unlike black phosphorus, $PdSe_2$ is air-stable, thus making it a promising candidate that will spark interest for 2D electronics.

Acknowledgement: This work was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility.

4:20pm 2D+MI-MoA-9 Hexagonal Boron-Carbon-Nitrogen – A Two-dimensional Direct Band Gap Semiconductor, Axel Enders, University of Bayreuth, Germany; S Beniwal, University of Nebraska - Lincoln; J Hooper, Jagiellonian University, Poland; D Miller, SUNY Buffalo; P Costa, University of Nebraska - Lincoln; S Liu, Boston College; C Sykes, Tufts University; E Zurek, SUNY Buffalo

Two-dimensional h-BCN, synthesized from the precursor molecule bis-BN cyclohexane on the (111) surfaces of Ir and Rh under ultrahigh vacuum, was investigated with a comprehensively suite of in-situ local probe microscopy and spectroscopy methods. The lattice structure of h-BCN is identical to that of graphene, with the graphenic sites occupied by atoms of boron, nitrogen and carbon. The film morphology exhibits a strain driven corrugation with a periodicity of 3.2 nm, reminiscent of published results for epitaxial graphene and h-BN. Due to differences in the epitaxial fit and interfacial interactions, this corrugation is more ordered on the Rh surface. Out of several candidate structures that are feasible by connecting the B₂C₂N₂ rings of the precursor molecules, the most likely film structure was established through combined density functional theory and X-ray photoelectron spectroscopy that studies the chemical environment of the film's atoms. Local tunneling spectroscopy shows an electronic band gap of h-BCN of 1.0 eV on Rh(111) and of 1.5 eV on Ir(111). On the basis of these measured gaps and the computationally predicted electronic band structure, especially a direct electronic band gap that is intermediate to those of the zero-band gap semiconductor graphene and the insulating h-BN, and the theoretical prediction that the band gap is dependent on the molecular tiling, it can be expected that the h-BCN layers are potentially exciting candidates for 2D electronic materials.

S. Beniwal, J. Hooper, D. P. Miller, P. S. Costa, G. Chen, S.-Y. Liu, P. A. Dowben, E. C. H. Sykes, E. Zurek, and A. Enders, “Graphene-like Boron–Carbon–Nitrogen Monolayers,” *ACS Nano*, vol. 11, no. 3, pp. 2486–2493, Mar. 2017.

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