Tuesday Evening Poster Sessions, October 22, 2019

2D Materials

Room Union Station AB - Session 2D-TuP

2D Poster Session

2D-TuP-1 Enhancement of Solid Solubility in 2D Alloys by Selective Orbital Coupling, ***Bing Huang***, Beijing Computational Science Research Center, China

Solid solubility (SS) is one of the most important features of alloys, which is extremely difficult to be largely tuned in the entire alloy concentrations by external approaches. As a result, some alloys, which were supposed to have promising physical properties, turn out to be much less useful because of their poor SS, e.g., the case for monolayer BNC alloys. The unavoidable phase separation in BNC alloys, caused by the unstable C-B and C-N wrong-bonds, has severely restricted their promising optoelectronic applications. In this talk, a mechanism of selective orbital coupling between wrong-bond states and surface states mediated by the substrate has been proposed to stabilize the wrong-bonds and in turn significantly enhance the SS of BNC alloys. Surprisingly, we demonstrate that the miscibility temperature of BNC grown on some specific substrates can be largely reduced, accompanied by the appearance of well-ordered ground-states. Interestingly, the homogenous BNC with fully tunable band gaps between 0 and 6 eV can be achieved under a low growth temperature of 1000 K. Our discovery provides a general concept to enhance the SS in monolayer alloys by selective orbital coupling.

2D-TuP-2 Black Phosphorus and Endohedral-Graphene Hybrids for Novel Optoelectronic Devices, *M Min,* ***Srishti Chugh***, *A Kaul,* University of North Texas

Among the various two-dimensional (2D) materials, graphene is a material of immense technological importance given its ballistic transport which provides opportunities for high-speed field-effect transistors (FETs). Other mono-elemental 2D materials such as black phosphorus (BP) provide a thickness-dependent, direct band gap ranging from ~ 0.3 eV in the bulk to ~1.5 eV in the monolayer limit. Here, in the first part of the work, we report on the integration of zero-dimensional materials with 2D graphene membranes to enhance the optoelectronic properties of the photodetectors. Quantum dot-graphene optoelectronic devices are discussed where mechanically exfoliated graphene flakes are used in a two-terminal device configuration. The zero-dimensional materials used in this work were cluster endohedral fullerenes, $Sc_3N@C_{80}$, and monometallic endohedral fullerene, $La@C_{82}$, based on their electron-accepting and electron-donating abilities, respectively. Temperature-dependent and wavelength-dependent optoelectronic properties of the 0D-2D graphene-based hybrids will be presented. In the second part of the work, we will also show the chemical exfoliation of BP to form optoelectronic devices with protecting layers to enhance the stability of the BP. Here, we present liquid exfoliation approaches to obtain BP by sonication in organic solvent such as 1-cyclohexyl-2-pyrrolidone (CHP), *N*-methyl-2-pyrrolidone (NMP) at ambient conditions. We compare the structural properties of black phosphorus through Raman Spectroscopy analysis, Photoluminescence (PL) and two-terminal electronic device measurements to demonstrate its enhanced device stability.

2D-TuP-3 Nitrogen-Doped Graphene on Cu(111): Edge-Guided Doping Process and Doping-Induced Variation of Local Work Function, *J Neilson, H Chinkezian, H Phirke, A Osei-Twumasi,* California State University, Northridge*; Y Li,* Peking University, China*; C Chichiri,* California State University, Northridge*; J Cho,* Myongji University, Korea*; K Palotás,* Hungarian Academy of Sciences, Hungary*; L Gan,* Peking University, China*; S Garrett, K Lau,* California State University, Northridge*;* ***Li Gao***, California State University Northridge

The nitrogen-containing sole precursor azafullerene has been used for the synthesis of nitrogen-doped graphene on the Cu(111) surface. The synthesis process, doping properties, and doping-induced variation of local work function of graphene have been studied on the atomic scale by combing scanning tunneling microscopy/spectroscopy, X-ray photoelectron spectroscopy, and density functional theory calculations. Most nitrogen dopants are at the edges of graphene islands and the graphene domain boundaries with the pyridinic configuration. Graphitic nitrogen dopants arrange into curved lines within graphene islands after multiple growth cycles, which results from a doping process guided by the edges of graphene islands. The doping-induced variation of local work function of the graphene surface has been measured on the atomic scale by recording spatially resolved field emission resonances. We find that the local work function strongly depends on the atomic bonding configuration and concentration of nitrogen dopants. The local work function decreases for graphitic nitrogen doping but increases for pyridinic nitrogen doping. This work provides new atomic-scale insights into the process for incorporating nitrogen atoms into the graphene lattice as well as the correlations between the type of nitrogen doping and the variation of local work function.

2D-TuP-4 Vibrational Progression of a Single Hydrocarbon Molecule on Graphene and Hexagonal Boron Nitride, ***Alexander Mehler***, *N Néel, J Halle,* Technische Universität Ilmenau, Germany*; M Bocquet,* École normale supérieure, PSL University, Sorbonne Université, CNRS, France*; J Kröger,* Technische Universität Ilmenau, Germany

Probing genuine molecular properties even after adsorption on a surface requires the efficient reduction of the molecule-surface hybridization. Two-dimensional materials, such as graphene, hexagonal Boron Nitride (hBN) and stackings thereof, are promising buffer layers to this end. Scanning tunneling microscopy and spectroscopy at low temperature is used to explore molecular orbitals and vibrational quanta of the hydrocarbon molecule DBP (Dibenzotetraphenylperiflanthen) on graphene and hBN with submolecular resolution. Independent of the metal substrate, Ir(111), Pt(111) and Ru(0001), vibrational progression in both DBP frontier orbitals is observed for graphene and hBN, albeit with different numbers of vibrational quanta involved. Density functional calculations unveil that symmetry matching of electronic and vibrational excitations supports the observation of vibrational progression. The lifetime of the vibronic levels can be tuned by the molecular environment of a single DBP as well as by using different kinds and numbers of buffer layers.

2D-TuP-5 Synthesis of Layered PdS_2 Film and Homo-junction Device Fabrication, *C Jong,* TSRI/NARL, Taiwan, Republic of China*; Y Yang,* NTNU, Taiwan, Republic of China*; M Le,* NTHU, Taiwan, Republic of China*; P Chen,* MUST, Taiwan, Republic of China*;* ***Chien-Bao Lin***, *P Chiu, C Hsiao,* TIRI/NARL, Taiwan, Republic of China

Lots of TMDs materials with fantastic properties have been widely discovered for electrical and optical device application. In order to replace current Si-based device several challenges should be overcame, including the 2D synthesis and patterning technique; heterojunction control between TMDs to TMDs, TMDs to dielectric film and TMDs to metallic film, doping technique and so on. Among them, MoS_2 and WSe_2 have shown their excellent electron and hole mobility in NFET and PFET evaluation. For electronic and photonic applications, a material existing air-stable, high carrier mobility, high on/off ratio, as well as a tunable band gap is far more desirable. Recent theoretical and experimental data show some noble chalcogenides can also form layered structures with S or Se atoms, like PdS_2 and $PdSe_2$[1-3]. Each Pd atom can bond to four S or Se atoms, respectively. Puckered $PdSe_2$ exhibit a widely tunable band gap that varies from metallic (bulk) to ∼1.3 eV (monolayer) and the field-effect transistors made from $PdSe_2$ reveal high electron field-effect mobility of ∼158 cm^2/Vs are presented [4]. Recently, Mahdi et al., [5] proposed a unique alternative to reduce contact resistance through the single material junction device scheme, that is, using a single material (PdS_2) in channel and S/D region. Monolayer PdS_2 was found to be semiconducting with a bandgap of 1.1 eV and became semi-metallic as bilayer. PdS_2 was also reported with a high electron mobility than MoS_2. However, not too much experimental works has been published yet in PdS_2 synthesis. To realize the reported device integration, the thickness control and sulfurization process are important. In our previous works [6-7], a possible approach in untra-thin and uniform 2D layer film synthesis was demonstrated combined with proposed ALE and sulfurization process.

In this study, the PdS_2 film synthesis and single material junction device fabrication will be performed. Pd film was sputtered onto SiO2/Si substrate for sulfurization. The PdS_2 film was obtained after sulfurization and the structure is verified [8]. The XRD, XPS and Raman spectrum are measured for microstructure evaluation. A lift -off process in channel and source and drain patterning was achieved. With the help of anisotropic etch in Pd film thin down, the desired thickness and wafer scale flatness was controlled. The etched thickness and surface roughness are monitored by AFM. Followed by the etch process, the etched samples were sulfurized for PdS_2 formation. After the sulfurization process the homo-junction device using a single material was fabricated and the electrical properties was characterization.

2D-TuP-6 NanoESCA III: Momentum Microscopy on 2D Materials, ***Marten Patt***, Scienta Omicron GmbH, Germany; *N Weber, M Escher, T Kuehn, M Merkel,* FOCUS GmbH, Germany

New 2D material classes including graphene, transition metal dichalcogenides (TMDCs) or 2D heterostructures based on TMDCs or graphene are nowadays a promising candidate to be used in future electronic devices. They are chemically versatile and thus predestined to tune their electronic structure for various applications (e.g. electronic, optoelectronic and spintronic).

To examine these materials, a fast band structure mapping in combination with a high lateral resolution in real-space and live view microscopy becomes essential. The band structure mapping is used to understand the electronic structure of new material combinations, while the real-space microscopy is needed to localize the crystals on the specimen, especially if they were produced by mechanical exfoliation or intercalation techniques [1].

The NanoESCA microscope allows to easily switch between the imaging of the real- and the momentum- space of photoemission electrons and is therefore predestined to examine novel 2D materials. In the so-called momentum microscopy mode, the NanoESCA acquires the band structure from a microscopic sample region of interest, which was beforehand defined in real-space.

We will show recent band-structure measurements of several TMDCs (see e.g. [2]) acquired with the instrument and discuss the latest technical improvements of the momentum microscopy technique with respect to 2D material characterization.

References

[1] Mattia Cattelan and Neil Fox, NanoMaterials 2018, 8, 284; doi:10.3390/nano8050284

[2] Ming-Wie Chen et al., npj 2D Materials and Applications (2018) 2:2 ; doi:10.1038/s41699-017-0047-x

2D-TuP-7 Shifting of Electronic States of Meso-tetrakis(pentafluorophenyl) Porphyrin Self-assembled Monolayers Due to Internal Molecular Structure, ***Jose Ortiz-Garcia***, *M Wolf, M Guberman-Pfeffer, J Gascon, D Thuita, C Brückner, R Quardokus,* University of Connecticut

Meso-tetrakis(pentafluorophenyl) porphyrin (T^FPP) self-assembled islands were imaged on Au (111) using an ultra-high vacuum scanning tunneling microscope (LT-UHV STM). A pulse-solenoid valve was used to deposit submonolayer coverage of T^FPP porphyrins on Au(111). A range of bias voltages were used to image occupied and unoccupied electronic states of T^FPP. Density functional theory (DFT) was used to calculate the spread in energy levels of both occupied and unoccupied molecular orbitals. We found that the spacing of the energy levels of electronic states shifts depending on the presence and location of hydrogens bonded to the inner nitrogens (locants 21-24).

2D-TuP-8 Reproducibility and Replicability in Science and Engineering: A Report by the National Academies, *T Winters,* ***Jennifer Heimberg***, National Academies of Sciences, Engineering, and Medicine

One of the pathways by which scientists confirm the validity of a new finding or discovery is by repeating the research that produced it. When a scientific effort fails to independently confirm the computations or results of a previous study, some argue that the observed inconsistency may be an important precursor to new discovery while others fear it may be a symptom of a lack of rigor in science. When a newly reported scientific study has far-reaching implications for science or a major, potential impact on the public, the question of its reliability takes on heightened importance. Concerns over reproducibility and replicability have been expressed in both scientific and popular media.

As these concerns increased in recent years, Congress directed the National Science Foundation to contract with the National Academies of Science, Engineering, and Medicine to undertake a study to assess reproducibility and replicability in scientific and engineering research and to provide findings and recommendations for improving rigor and transparency in research.

The committee appointed by the National Academies to carry out this task included individuals representing a wide range of expertise: methodology and statistics, philosophy of science, science communication, behavioral and social sciences, earth and life sciences, physical sciences, computational science, engineering, academic leadership, journal editors, and industry expertise in quality control. Individuals with expertise pertaining to reproducibility and replicability of research results across a variety of fields were included as well.

This poster will present the committee's approach to the task and highlights from its findings, conclusions, and recommendations related to factors that influence reproducibility, sources of replicability, strategies for supporting reproducibility and replicability, and how reproducibility and replicability fit into the broader framework of scientific quality and rigor.

2D-TuP-9 Structural and Electronic Properties of Native Point Defects in $MoTe_2$, ***Ziling Deng***, *S Mueller, W Windl, J Gupta,* The Ohio State University

We performed density functional theory(DFT) calculation to studied the structural and electronic properties of native point defects in $MoTe_2$. Various kinds of defects, e.g., vacancies, antisites with different charge states will be considered. With DFT, we will predict the constitutional defects with the lowest formation energies for all systems in Mo-rich, Te-rich and stoichiometric conditions as well as their dominated charge states. Additionally, the resulting output of our theoretical atomic scale model based on DFT-calculation will be used to simulate Scanning Tunneling Microscopy
[https://en.wikipedia.org/wiki/Scanning_tunneling_microscope](STM)
images to allow for comparison with experimental STM images. This study will provide an effective method to study the defects in $MoTe_2$ systems, with the comparison with experiments, the results will shed new light on the defect studying in $MoTe_2$.

MoTe2, a two-dimensional(2D) layered material has recently attracted much attention due to its excellent electronic properties. Intrinsic defects are commonly observed in MoTe2 growth, which would have a significant impact on the physical, optical, thermal, and electrical properties of the material. However, studying the atomic structure of intrinsic defects in this 2D materials is difficult since they damage quickly under the intense electron irradiation in TEM. To overcome this, we have performed a joint study between STM measurements and DFT calculations to identify the atomic structure and electronic nature of native point defects in MoTe2. We constructed analytical model from DFT and studied the structural and electronic properties of those defects. In order to understand the formation of defects and their atom-scale dynamics in MoTe2, we will use DFT to predict the constitutional defects with the lowest formation energies as well as their dominated charge states in Mo-rich, Te-rich and stoichiometric conditions to determine the necessary chemical potentials for all systems of MoTe2. Additionally, theoretically simulated STM images generated by density functional theory were used to compare with experimental STM data to enable us to assign structure of a number of defects observed during experiments.

This study provides an effective method to study the defects in $MoTe_2$ systems by presenting results for the energetics of native point defects in MoTe2. Base on our calculation, the formation energies and charged states of the vacancies and antisites will be determined, moreover, the simulated simulated STM images allow for the identification of structural defects of MoTe2 observed in the experiment.

2D-TuP-10 A Role of Au Atoms on Oxidized Black Phosphorus; Study using Scanning Photoelectron Microscopy, *D Kim, H Choi,* ***Jaeyoon Baik***, Pohang Accelerator Laboratory, Republic of Korea

We investigated oxygen reduction of black phosphorus(BP) using scanning photoemission electron spectroscopy. In spite of many effort of realizing ultra-thin film transistor of 2-dimensional atomic material of BP, inherent limitation in the transfer method such as oxidation, has not allowed application in real devices. Therefore, it is necessary to study the development of methods to prevent oxidation or reduction through the post-processing. However, such studies are very important to observe chemical composition changes using XPS, but there are other limitations in investigating based on flakes of the BP in um-size using general XPS . In this work, we observed Au atom, which deposited on BP, could play a role of catalyst reducing the oxidation on the top layers of BP. Using SPEM analysis method with 200nm spatial resolution, we verified the reduction mechanism of the um-size flake BP. As a result, we could observe that oxygen in the BP oxide disappeared through the Au atoms. Therefore, this can be applied to BP's Oxide Removal and Thickness Control technology and is expected to provide useful information for future application of the element.

References

[1] Zehua Hu et al., Nanoscale (2018) 10, 21575 ; doi:10.1039/c8nr07395c.

[2] Hao Huang et al., npj 2D Materials and Applications (2017) 1:20 ; doi:10.1038/s41699-017-0022-6.

2D-TuP-11 Growth and Electrical, Nano-Optical Characterization of semiconducting MoS_2/WS_2 in-plane Heterostructures, ***Sourav Garg**, P Kung, S Kim,* The University of Alabama*; A Krayev,* Horiba Scientific, Novato

In-plane heterojunctions of atomic-thick (2D) semiconductors (MoS_2/WS_2) are novel structures that can potentially pave the way for efficient ultrathin and flexible optoelectronics, such as light sources and photovoltaics. Such heterostructures (HS) are very rare and not much is known about their characteristics. They can only be achieved through a synthetic growth process such as chemical vapor deposition (CVD). This is unlike vertical heterostructures, for which the materials can be mechanically stacked one layer on top of the other. The CVD growth of in-plane heterostructure is a thermodynamically driven process and presents a number of challenges to control the vapor pressure of the precursors. Additionally, new analytical tools need to be developed in order to gain access to and understand the physical properties of these HS.

Here, we report a one-step CVD growth of monolayer (1 nm) thick MoS_2/WS_2 in-plane heterostructures. We have characterized their morphological and optical properties using micro-Raman and photoluminescence spectroscopy. Kelvin probe force microscope was used to extract the surface potential profile across the MoS_2/WS_2 heterojunction boundary, which was then used to gain access to fundamental semiconductor heterostructure parameters such as depletion layer width and built-in field across the MoS_2-WS_2 interface. In-addition more rigorous study of heterostructures interface by tip enhanced PL (TEPL) had been performed.

2D-TuP-12 Identifying Key Parameters for the Uniformity of Nanopatterning on 2D Highly Oriented Pyrolytic Graphite Layers, ***James Su**,* Taiwan Instrument Research Institute, National Applied Research Laboratories, Taiwan, Republic of China

Demonstrations of local anodic oxidation nanopatterning on 2D highly oriented pyrolytic graphite (HOPG) layers were performed by adopting a conductive atomic force microscope (CAFM). Parameters such as environmental humidity, temperature, tip bias, tip velocity, set-point and apex curvature were evaluated for the uniformity of nanopatterning on HOPG. The patterns created by this method varied as the tip bias increases up to 6.8 V or tip force over 96 nN.

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