

Thursday Evening Poster Sessions

2D Materials Focus Topic

Room: Hall 3 - Session 2D-ThP

2D Materials Focus Topic Poster Session

2D-ThP1 Spin-Orbit Coupling in the Band Structure of Monolayer WSe₂(0001), *Iori Tanabe*, University of Nebraska - Lincoln, *D. Le*, University of Central Florida, *A.V. Barinov*, Sincrotrone Trieste, Italy, *E. Preciado*, *M. Isarraraz*, University of California - Riverside, *T. Komatsu*, University of Nebraska - Lincoln, *L. Bartels*, University of California - Riverside, *T.S. Rahman*, University of Central Florida, *P.A. Dowben*, University of Nebraska - Lincoln

WSe₂ and the related metal dichalcogenides MX₂ (with M = V, Mo, W, Ta and X = S, Se, Te) are layered structures that in each plane consist of a hexagonal honeycomb lattice reminiscent of graphene or graphite. WSe₂ is a semiconductor, rather than a gapless semiconductor (like graphene) or semimetal, and is expected to have applications for new spintronic devices where spin-orbit coupling might play a valuable role. Here, we used high-resolution angle resolved photoemission spectroscopy (ARPES) and inverse photoemission spectroscopy (IPES) to map out the electronic band structure of single-layer WSe₂. The splitting of the top of the valence band due to spin-orbit coupling was found to be 513±10 meV, far larger than that for MoS₂. As expected the top of the valence band is at K. Overall, density functional theory (DFT) calculations were in excellent agreement with the ARPES results, and we have verified that the few discrepancies between theory and experiment were not due to the effect of strain. Cobalt on WSe₂ is seen to have a very complex interface, with strong interactions, as seen in the changes to the experimental electronic structure. Without the complexity of a metal adlayer, WSe₂ is seen to be routinely Se rich and should thus be reliably p-type.

2D-ThP2 Ferroelectric Control of Monolayer MoS₂ via Direct Single-Layer Growth on LiNbO₃, *Ariana Nguyen*, *E. Preciado*, *V. Klee*, *D. Sun*, *I. Lu*, *D. Barroso*, *L. Bartels*, UC Riverside

We present the direct chemical vapor deposition (CVD) growth of monolayer molybdenum disulfide (MoS₂) onto periodically poled lithium niobate. Single-layer MoS₂ displays a preference for the ferroelectric domains polarized “up” with respect to the surface. This may offer the possibilities of templated growth of TMD films using the substrate ferroelectric polarization as a pattern. Piezoresponse force microscopy reveals that the MoS₂ film maintains the substrate polarization on the “up” domains while partially quenching it on the “down” domains. Electrical transport measurements suggest the ability to invert the single-layer CVD MoS₂ majority charge carrier via gating depending on the domain orientation of the periodically poled lithium niobate substrate.

2D-ThP4 Thermally Conductive Graphene-Polymer Composites, *Michael Shtein*, *O. Regev*, Ben Gurion University, Israel

The rapidly increasing device densities in electronics dictate the need for efficient thermal management. If successfully exploited, graphene, which possesses extraordinary thermal properties, can be commercially utilized in polymer composites with ultrahigh thermal conductivity (TC). The total potential of graphene to enhance TC, however, is restricted by the large interfacial thermal resistance between the polymer mediated graphene boundaries. We report a facile and scalable dispersion of commercially available graphene nano platelets (GnPs) in a polymer matrix, which formed composite with an ultra-high TC of 12.4 W/mK (vs. 0.2 W/mK for neat polymer).[1] This ultra-high TC was achieved by applying high compression forces during the dispersion resulting in gap closure between adjacent GnPs with large lateral dimensions and low defect densities. We also found strong evidences for the existence of a *thermal percolation threshold*. Finally, the addition of electrically insulating nano-boron nitride to the thermally conductive GnP-polymer composite significantly reduces its electrical conductivity (to avoid short circuit) and synergistically increases the TC. The efficient dispersion of commercially available GnPs in polymer matrix provides an ideal framework for substantial progress toward large-scale production and commercialization of GnP-based thermally conductive composites.

Reference: Shtein M., Nadiv R., Buzaglo M., Kahil K. and Regev O., Thermally conductive graphene-polymer composites: size, percolation and synergy effects, *Chemistry of Materials*, 2015, 27, 2100–2106 .

2D-ThP5 Low Temperature Raman and Photoluminescence Measurements of MoS₂ Layer Grown by Chemical Vapor Deposition, *Barbara Nichols*, U.S. Army Research Laboratory, *R. Ghosh*, *S.K. Banerjee*, University of Texas at Austin

The temperature-dependent Raman spectroscopy and photoluminescence mapping measurements of molybdenum disulfide (MoS₂) layers grown on silicon oxide (SiO₂) by chemical vapor deposition were performed. As grown, the MoS₂ monolayers are shaped as either hexagons or triangles with smaller dendritic adlayers randomly distributed throughout the layer. Specifically, Raman and PL mapping of a 20 micron wide hexagon was performed at room temperature in air and in vacuum. In both air and vacuum, the Raman A_{1g} – E_{2g} separation was wider for the dendritic adlayers than for the monolayer MoS₂ as well as a decreased PL intensity was observed for the dendrites when compared to the monolayer. Raman and PL mapping of the MoS₂ hexagon revealed these trends remained as the temperature was decreased from room temperature to 4 K. At 4 K, differences between the dendrites and the monolayer MoS₂ were mainly observed by the PL measurements. PL peak position shifts as much as 15 meV and peak shapes were observed for the A and B exciton transitions.

2D-ThP6 CVD Growth of Single-Layer TMD Films Onto Pre-Fabricated Substrate Structures, *B. Davis*, *E. Preciado*, *V. Klee*, *A. Nguyen*, *I. Lu*, *D. Barroso*, *S. Naghibi*, *I. Liao*, *G. von Son*, *D. Martinez-Ta*, *Ludwig Bartels*, UC Riverside

We demonstrate the growth of transition metal dichalcogenides (TMD) single-layer films through chemical vapor deposition (CVD) onto pre-fabricated patterns on SiO₂/Si surfaces. For an ultimate technological application of single-layer TMD films, they need to be integrated into lithographic structures on SiO₂/Si substrates; exfoliation and/or transfer are not suitable or scalable techniques. The comparatively low growth temperatures of TMD films (about 700°C) compared to graphene (about 1000°C) is a crucial advantage of the former, as SiO₂/Si features can sustain the growth temperature. Here we offer examples of how pre-fabricated patterns can control the growth of TMD films, and how the latter arrange themselves into former to offer features (e.g., natively suspended material) that is typically not available directly from growth onto conventional flat substrates. We explore the electrical and optical properties of single-layer growth on substrates with holes, pillars, and trenches.

2D-ThP7 MoS₂ Thin Films Deposited by Chemical Bath Deposition on Si and Glass Substrates, *D.E. Perez-Barragan*, Escuela Superior de Ingenieria Quimica e Industrias Extractivas-IPN, Mexico, *A. Garcia-Sotelo*, *E. Campos*, Cinvestav-IPN, Mexico, *Orlando Zelaya-Angel*, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, *M. Melendez-Lira*, Cinvestav-IPN, Mexico

Even when the increasing interest in MoS₂ is driven by their properties as a 2D material, the deposit of MoS₂ films using low cost techniques is interesting and allows to explore the feasibility to find routes to produce low cost materials capable to improve photovoltaic structures, etc. The results of the deposit by chemical bath deposition of MoS₂ films employing Si and glass substrates are presented. Two precursor were employed: Ammonium molybdate (NH₄)₂MoO₄ and Ammonium molybdate tetrahydrate (NH₄)₆Mo₇O₂₄ · 4H₂O. It was found that the first precursor is adequate to obtain amorphous MoS₂ films on glass while the second allows to obtain amorphous films on silicon.

The samples crystallized after a thermal annealing process carried out at 300 °C. UV-Vis spectroscopy indicated a blue-shift in the absorption edge from the MoS₂ bulk value, probably related to the film thickness. Samples were characterized also by XPS, Raman and AFM. The results are discussed in terms of the structural characteristic of the films and the interaction with the substrate.

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2D-ThP8 Development of Arrays of Field Effect Transistors Based on CVD Graphene and TaN as Metal Electrode, *Aline Pascon*, UNICAMP, Brazil, *C.C. Silva*, University of Campinas, Brazil, *J.F. Souza*, UNICAMP, Brazil, *L.T. Kubota*, University of Campinas, Brazil, *L.R.C. Fonseca*, *J.A. Diniz*, UNICAMP, Brazil

Since graphene was successful isolated for the first time by microcleaving of graphite [1], this material has attracting a significant attention of all scientific community, mainly due to its outstanding electronic properties, making it an ideal material to replace the silicon in the traditional FETs. However, the implementation of graphene in the development of FETs has two major issues that should be overcome. The first is that graphene obtained from microcleaving or exfoliation of graphite, does not feature like

a scalability technique to be employed in the fabrication of arrays of FETs. The second issue is related with the high contact resistance that appears in the interface metal/graphene. In order to replace the silicon by the graphene as a channel material, a suitable contact with electrodes is required. Aiming to overcome the related issues, herein we have addressed the implementation into arrays of FETs by large area of monolayer graphene produced by the CVD process. Furthermore, we evaluated the effects of the replacement of the conventional, non-refractory metallic electrodes such as Ti/Au or Ti/Pd for the refractory metallic electrodes, such as tantalum nitride (TaN) that has a work function similar to graphene reducing the barrier between metal and graphene.

The CVD graphene was grown based on the procedure proposed by Ruoff and coworkers [2]. This graphene film was transferred on FETs where 22 nm TaO₂ was used as gate dielectric, in just one step, homogenous and free from PMMA residues or other contamination. The Raman spectra obtained from different areas of the graphene displays a typical G peak at 1587 cm⁻¹, free of defects and a 2D peak at 2684 cm⁻¹, indicating a monolayer of graphene [3].

After the transferring process, the graphene was isolated between the source and drain TaN electrodes due to the photolithography step followed by the oxygen plasma etching, to remove the graphene in the outside area, creating a contact with the electrodes, similar to the dielectric gate. All this process was carried out directly on a die of 2.5 cm² containing four arrays with 300 FETs each. The latter two processes define the active region of the device, where the electronic transport will occur through the graphene monolayer.

Measurements of electrical properties, with transconductance of 3 mS and contact resistance of 3 kΩ indicate that our devices can achieve high performance, while allows fabricating a massive number of FET-Graphene devices through a simple, fast and scalable approach.

References

- [1] K. S. Novoselov et al, Science , 666 (2004).
- [2] Xuesong Li, et al., Science **324**, 1312 (2009).
- [3] A. C. Ferrari et al., PRL **97**, 187401 (2006) .

2D-ThP11 Conductance-Based Structural Characterization of Hybrid, 2-Dimensional, Molecule-Nanoparticle Arrays, Joshua Hihath, C.E. McCold, Q. Fu, University of California, Davis, J.Y. Howe, Hitachi High-Technologies Corporation

Molecule-nanoparticle hybrid systems have emerged as promising materials for applications ranging from chemical sensing to nanoscale electronics. However, creating reproducible and repeatable 2-dimensional composite materials with precise electronic properties has remained an important challenge to the implementation of these meta-materials. Understanding the sources of variation that dominate the charge transport properties of these systems is essential for the advancement of nanoparticle-array based devices. In this work, we use a combination of charge-transport measurements, electron microscopy, optical characterization, and chemical ligand exchange to determine the role of morphology, structure, and array interconnection on the charge transport properties of 2-dimensional, monolayer arrays of molecularly-interlinked gold nanoparticles. Using these techniques we are able to determine the role of assembly-dependent, particle dependent, and molecule dependent defects on the conductivities of the monolayer films. These results demonstrate that micron-scale assembly processes dominate the dispersion of the conductance values, and result in order-of-magnitude differences in the conductance values, while nanoscale properties related to the nanoparticle and ligand features dictate the mean value of the conductance. By performing a systematic study of the conductance of these arrays as a function of nanoparticle size we are able to extract the carrier mobility for specific molecular ligands. We show that nanoparticle dispersion correlates with the void density in the array, and that because of this correlation it is possible to accurately determine the void density within the array directly from conductance measurements. These results demonstrate that conductance-based measurements can be used to accurately and non-destructively determine the morphological and structural properties of these hybrid arrays, and thus provide a characterization platform that helps move 2-dimensional nanoparticle arrays toward robust and reproducible electronic systems. Based upon this understanding, it is then possible to control the conductance values of the hybrid arrays by tuning both the distance between nanoparticles, and the conjugation of the molecules interlinking the nanoparticles. This control allows the conductance of the 2D films to be tuned over a range of ~7 orders of magnitude.

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