2D Materials Focus Topic
Room 103B - Session 2D-TuA

Novel Quantum Phenomena in 2D Materials

Moderators: Yoshi Iwasa, University of Tokyo, Japan, Kristian Thygesen, Technical University of Denmark

2:20pm **2D-TuA1 Time-dependent Density-functional Theory Simulation of Local Currents in Pristine and Single-defect Zigzag Graphene Nanoribbons**, ***S He***, *A. Russakoff, Y. Li, K. Varga,* Vanderbilt University

The spatial current distribution in H-terminated zigzag graphene nanoribbons (ZGNRs) under electrical bias is investigated using time-dependent density-functional theory solved on a real-space grid. A projected complex absorbing potential is used to minimize the effect of reflection at simulation cell boundary. The calculations show that the current flows mainly along the edge atoms in thehydrogen terminated pristine ZGNRs. When a vacancy is introduced to the ZGNRs, loop currents emerge at the ribbon edge due to electrons hopping between carbon atoms of the same sublattice. The loop currents hinder the flow of the edge current, explaining the poor electric conductance observed in recent

3:00pm **2D-TuA3 Studies of Conductance in Graphene Defects and Junctions using Complex-Injecting Potentials and TDDFT**, ***Cody Covington***, *K. Varga,* Vanderbilt University

In order create nanoscale electronic devices, there is a need for making high quality electrical connections between functional regions or specific defects[1]. However, connecting dissimilar materials such as graphene and metals[2] may pose complications from differing densities of states and work functions, and predicting how the system is effected computationally can be challenging given the system size. To address these challenges, studies of the electrons flow through heterogeneous material junctions, using complex potentials on a real-space grid and Time-Dependent Density Functional Theory have been performed. By confining an electron into the conduction band at a single point and propagating the system in time, the wavefunction for the system in a specific conducting state can be solved. Considerations for junctions and use of injecting and absorbing potentials in regions of diminished electron density will be presented.

[1] J. Lahiri, Y. Lin, P. Bozkurt, I.I. Oleynik, M. Batzill, An extended defect in graphene as a metallic wire, Nat Nano, 5 (2010) 326-329.

[2] F. Xia, V. Perebeinos, Y.-m. Lin, Y. Wu, P. Avouris, The origins and limits of metal-graphene junction resistance, Nat Nano, 6 (2011) 179-184.

3:20pm **2D-TuA4 Excited Biexcitons in Two-Dimensional Transition Metal Dichalcogenides**, ***Daniel Kidd***, *D. Zhang, K. Varga,* Vanderbilt University

Recently, experimental measurements and theoretical modeling have been in a disagreement concerning the binding energy of biexctions in transition metal dichalcogenides. While theory predicts a smaller binding energy (~20 meV) that is lower than that of the trion, experiments find values much larger (~60 meV), actually exceeding those for the trion. In this work, we show that there exists an excited state of the biexciton which yields binding energies that match well with experimental findings and thus gives a plausible explanation for the apparent discrepancy. Ground and excited states of the five-body exciton-trion are also investigated and shown to be bound.

4:20pm **2D-TuA7 Electron Talbot Effect on Graphene**, ***Jorge Salas***, Vanderbilt University

The Talbot effect for a graphene sheet as a grating, using electron matter waves, is simulated using density functional theory and solving the Helmholtz equation. The obtained Talbot images show focusing effects suggesting possible applications for reshaping electron wave-packets and interferometry [1].

[1] Salas, J. A., Varga, K., Yan, J.-A. & Bevan, K. H. Electron Talbot effect on graphene. Phys. Rev. B 93, 104305 (2016).

4:40pm **2D-TuA8 Femtosecond Hot Electron-Phonon Interactions of Single Layer Graphene and the undelying Substrate**, ***Zina Jarrahi***, *J.L. Davidson, N.H. Tolk,* Vanderbilt University

We study the effect of substrate on the femtosecond transient electron and phonon dynamics of single layer graphene transferred on finely polished diamond, sapphire and quartz. Through a comprehensive set of fluence and energy dependent ultrafast optical conductivity measurements, we show that the temporal evolution of the hot carriers in graphene, differ *significantly* depending on the underlying substrate. We observe much faster(slower) relaxation and less(more) pronounced band filling dynamics for graphene on diamond(quartz). We demonstrate that the differences in the temporal evolution of the carrier temperature and inter/intraband transition interplay, cannot be accounted for by invoking the different static Fermi-levels of graphene on each substrate. These substrate-dependent dynamics are explained, using a multi-channel cooling picture, involving surface phonons of the substrate, intrinsic optical phonons of graphene, their competing scattering rates, phonon frequencies and the varying Fröhlich coupling strength of the different substrates. In this regard, the sub nm roughness of our studied substrates, enable a strong coupling between the phototexcited carriers in graphene and the surface vibrational modes of the polar substrates. We observe an increase in the carrier relaxation times as photoexcited carrier density is increased. This further confirms the existence of an additional relaxation mechanism through the substrate that competes with the intrinsic phonons of graphene to not only reduce the electron temperature but also carrier and optical phonon lifetimes. These results offer significant potential to selectively activate the desired energy relaxation channels in graphene and tune the carrier and optical phonon lifetimes, by simply varying the substrate and fluence regime. This knowledge will pave the road towards designing graphene-based (opto)electronics with highly tailored functionalities suited for specific device requirements.

5:00pm **2D-TuA9 New Opportunities in Two-Dimensional Material Research**, ***Yuanbo Zhang***, Fudan University, China **INVITED**

Two-dimensional (2D) atomic crystals, best exemplified by graphene, have emerged as a new class of material that may impact future science and technology. The reduced dimensionality in these 2D crystals often leads to novel material properties that are vastly different from that in the bulk. We refer to such a recurring scheme as “less is different”. In this talk I will illustrate this scheme with two 2D materials that we found particularly interesting – black phosphorus and 1T-TaS_2. These two layered materials have vastly different properties. Black phosphorus is a 2D semiconductor, and its superior material quality has recently enabled us to observe the quantum Hall effect. 1T-TaS_2, on the other hand, is a metal with a rich set of charge density wave phases. We explore their electronic properties while the doping and dimensionality of the 2D systems are modulated.

5:40pm **2D-TuA11 Ultrafast Carrier Dynamics in the Quasi-2D Metal Dichalcogenide SnS_2**, ***Oliver Monti***, *C. Eads, D. Bandak,* University of Arizona*; D. Nordlund,* SLAC National Accelerator Laboratory*; M. Neupane,* US Army Research Laboratory

We use soft x-ray resonant photoemission and core-hole-clock spectroscopy to investigate the ultrafast carrier dynamics in SnS_2. We show that carriers delocalize on a time-scale of a few hundred attoseconds near the conduction band minimum, but remain localized over an order of magnitude longer in higher lying bands. On the basis of density functional theory calculations we are able to show that this is consistent with the 2D nature of SnS_2. Moreover, we show that these experiments map the wavefunction in the unoccupied bands. Our measurements represent the first of their kind on the carrier dynamics in such materials.

6:00pm **2D-TuA12 MBE Growth of WTe_2 for Novel Electronic and Topologically Protected Devices**, ***Lee Walsh***, *R. Yue, A.T. Barton, H. Zhu, L. Cheng, R. Addou, J. Hsu, J. Kim, M. Kim,* University of Texas at Dallas*; L. Colombo,* Texas Instruments*; R.M. Wallace, C.L. Hinkle,* University of Texas at Dallas

Transition metal dichalcogenides (TMDs) are 2D materials which belong to a class known as van der Waals materials where the adjacent layers are held together by weak van der Waal’s interactions and, in principle, have no surface dangling bonds, which permits a relaxed growth requirement in terms of lattice matching. This relaxed lattice-matching criteria allows us to couple these materials based primarily on their band alignment and electronic properties. WTe_2 is a TMD with an equilibrium structure in the distorted octahedral (1T’) phase. This 1T’ phase of WTe_2 is a semi-metal and hence may be implemented as a 2D metal in an all-2D heterostructure for new devices. Monolayer 1T’ WTe_2 has been separately predicted to be a Weyl semi-metal and to behave as a relatively wide bandgap (>0.1 eV) topological insulator, possessing helical edge states which have a number of interesting properties including time reversal symmetry, spin-momentum locking, and ballistic transport[1,2]. The trigonal prismatic (2H) phase of WTe_2 is viewed as an integral part of the tunnel field effect transistor (TFET) device due to its bandgap and effective mass and has been theoretically predicted to provide low power operation and sub 60 mV subthreshold swing. WTe_2 is truly a remarkable material with intriguing electronic properties owing to its strong spin-orbit coupling and layered crystal structure.

In this work, we demonstrate the first report of WTe_2 growth by molecular beam epitaxy (MBE) on a variety of substrate materials (Bi_2Te_3, MoS_2, and graphite). We will discuss the optimal MBE growth conditions (substrate temperature, flux rates etc.) along with in-depth structural and chemical characterization of the resultant single crystal thin films. Characterization was conducted via reflection high energy electron diffraction, transmission electron microscopy, scanning tunneling microscopy/spectroscopy, atomic force microscopy, X-ray photoelectron spectroscopy, and Raman spectroscopy. Challenges associated with Te incorporation and simple device and transport measurements will be presented.

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1. A. A. Soluyanov et. al, *Nature***527**, 495 (2015).

2. X. Qian et. al, *Science***346**, 1344 (2014).

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