PCSI

Room Canyon/Sugarloaf - Session PCSI-1ThM

2D Materials - Strain and Heterostructures

Moderator: Joshua Robinson, The Pennsylvania State University

8:30am **PCSI-1ThM-1 Electron Transport in Strain-Engineered Graphene**, ***Nadya Mason,*** University of Illinois at Urbana Champaign **INVITED**

There is wide interest in using strain-engineering to modify the physical properties of 2D materials, for both basic science and applications. Deformations of graphene, for example, can lead to the opening of band gaps, as well as the generation of pseudo-magnetic fields and novel electronic states. We demonstrate how controllable, device-compatible strain patterns in graphene can be engineered by depositing graphene on corrugated substrates. We discuss several techniques for creating corrugated substrates [1,2], focusing on periodic spherical curvature patterns in the form of closely packed nanospheres. We show how the smaller nanospheres induce larger tensile strain in graphene, and we explain the microscopic mechanism of this [3]. We also present experimental results demonstrating how a nearly periodic array of underlying nanospheres creates a strain superlattice in graphene, which exhibits mini-band conductance dips and magnetic field effects that depend on the magnitude of induced strain [4]. This control of the strain degree of freedom provides a novel platform both for fundamental studies of 2D electron behavior and for prospective applications in 2D electronic devices.

9:10am **PCSI-1ThM-9 UPGRADED: Revealing Exciton Masses and Dielectric Properties of Monolayer Semiconductors with High Magnetic Fields**, ***Mateusz Goryca,*** *J Li, A Stier,* Los Alamos National Laboratory*; T Taniguchi, K Watanabe,* National Institute for Materials Science, Japan*; E Courtade, S Shree, C Robert, B Urbaszek, X Marie,* Universite de Toulouse, INSA-CNRS-UPS, LPCNO, France*; S Crooker,* Los Alamos National Laboratory

In semiconductor physics, many of the essential material parameters relevant for optoelectronics can be experimentally revealed via optical spectroscopy in sufficiently large magnetic fields. For the new class of monolayer transition-metal dichalcogenide (TMD) semiconductors, this field scale can be substantial – many tens of teslas or more – due to the relatively heavy carrier masses and the very large electron-hole (exciton) binding energies. For that reason many fundamental parameters of TMDs were – up to now – still assumed from density functional theory calculations and have not been experimentally measured.

Here we report circularly-polarized absorption spectroscopy of the monolayer semiconductors MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 in very high magnetic fields up to 91 T. By encapsulating exfoliated monolayers in hexagonal boronnitride (hBN), we achieve very high optical quality structures that allow to follow the diamagnetic shifts and valley Zeeman splittings of not only the 1*s* ground state of the neutral exciton but also its excited 2*s*, 3*s*, ..., *ns* Rydberg states. The energies and diamagnetic shifts provide a direct determination of the effective (reduced) exciton masses and the dielectric properties of these monolayer semiconductors. Unexpectedly, the measured exciton masses are significantly heavier than predicted for Mo-based monolayers. Moreover, we also measure other important material properties, including exciton binding energies, exciton radii, and free-particle bandgaps. These results provide essential and quantitative parameters for the rational design of optoelectronic van der Waals heterostructures incorporating 2D semiconductor monolayers.

9:30am **PCSI-1ThM-13 Optical Determination of Ice-Induced Interfacial Strain on Single-Layer Graphene**, ***Subash Kattel,*** *J Murphy, S Pasco, J Ackerman, V Alvarado, W Rice,* University of Wyoming

Ice formed on a material creates a strain that is indicative of its adhesive strength with another material. Previous determinations of ice adhesion strength, a critical parameter for understanding icing physics, have proven to be highly dependent on experiment-specific conditions, such as surface roughness, icing conditions, water purity, etc. In this work, we use Raman spectroscopy to contactlessly and non-destructively measure temperature-dependent ice-induced strain for the first time. To isolate the ice-material interface, we probe the vibrational modes of single layer graphene (SLG) from 20°C to -30°C with and without ice as shown in Figure 1(a). Along with the well-known temperature-dependent Raman shift of SLG, a clear, ≈2 cm^{-1} change in the 2D-frequency (2650 cm^{-1}) developed upon ice formation is shown in Figure 1(b). We found this change in the Raman shift occurred even between supercooled water and ice at the same temperature. This small, change in the Raman shift of SLG corresponds to a 0.013% strain, which we show through spatial Raman mapping has a rich variation over the ice-SLG interface, as depicted in Figure 2. This point-by-point spatial mapping of the ice-induced strain enables precise correlation with surface roughness evaluation methods and theoretical models . Our results demonstrate that vibrational spectroscopy of 2D monolayers can precisely and locally measure strain at ice-material interfaces.

9:35am **PCSI-1ThM-14 UPGRADED: Electron Pairing by Remote-Phonon Scattering in Oxide-Supported Graphene**, *D Shin,* The University of Texas*; M Fischetti,* The University of Texas at Dallas*;* ***Alex Demkov,*** The University of Texas

Using first principles calculations we have shown that placing graphene on a (111)-oriented perovskite $SrTiO_3$ (STO) surface provides a possible doping mechanism [1]. Further theoretical analysis presented here suggests that coupling of electrons in graphene to interfacial hybrid plasmon/optical modes via remote-phonon scattering may result in an effective attractive electron-electron interaction that, in turn, could lead to electron pairing and superconductivity [2]. Specifically, we consider top-gated graphene supported by STO as shown in Fig.1. Using the full dynamic polarizability within the random phase approximation (RPA) for the entire system (including the hybrid modes arising from the coupling of the graphene plasmons to the optical phonons of the STO substrate and gate insulator), we estimate the superconducting transition temperature in the strong-coupling limit. In Fig. 2, we show the estimated superconducting critical temperature as a function of carrier density for different oxide thicknesses. As the carrier density increases, the critical temperature increases. The critical temperature is higher in the system of thicker HfO_2 oxide since the electron-IPP interaction is stronger with thicker top-gate oxide.

Figure 1**.** Schematic of a model used in our calculation. Here the STO substrate is assumed to be semi-infinite and the graphene layer is laterally infinite in the vacuum region between HfO_2 and STO.

Figure 2. Estimated superconducting critical temperature as a function of carrier density and the two indicated values of the oxide thickness in the strong-coupling limit.

[1] D. Shin and A. A. Demkov, Phys. Rev. B **97**, 075423 (2018).

[2] D. Shin, M. V. Fischetti, and A. A. Demkov, Phys. Rev. B **100**, 125417 (2019).

+ Author for correspondence: demkov@physics.utexas.edu

9:55am **PCSI-1ThM-18 Modeling of Interfaces in All-Solid-State Li-ion Batteries**, ***Yue Qi,*** Michigan State University **INVITED**

Paring solid electrolytes with Li metal anode and high voltage cathodes form promising all-solid-state Li-ion batteries with higher energy density and ultimately safety. With the rapid development of fast Li-ion conducting solid electrolytes, the major bottleneck for all-solid-state Li-ion batteries lies at the high interfacial resistance and Li dendrite growth. This talk will focus on new mechanism understanding obtained by atomisticly-informed multi-scale modeling approaches.

The high interfacial resistance is due to two main factors: physical contact and chemical effect. The chemical effect was captured by a new density functional theory (DFT) based model, which predicts the potential map inside a solid-state battery and determines the potential drop, electrostatic dipole, and space-charge layer at the electrode/solid-electrolyte interface.[1] This new physics insight unified the seemingly contradictory experimental observations and led to new device design rules to promote interfacial ion transport in future solid-state batteries.[2] The physical contact was described by combining contact mechanics and 1D Newman battery model. The model suggested how much pressures should be applied to recover the capacity drop due to contact area loss.

To simulate Li dendrite growth inside polycrystalline solid electrolytes, we coupled DFT calculations with the phase-field method. This model successfully explained the experimentally observed dendrite intergranular growth and revealed that the trapped electrons at grain boundaries and surfaces may produce isolated Li-metal nucleation, leading to a sudden increase of Li-dendrite penetration depth. Based on the model, we developed new dendrite resistant criteria by comparing the basic material properties for a number of solid electrolytes including LLZO, Li_3PS_4, LATP, and LiPON. [3][4]

These modeling advancements will be integrated into a new framework to guide the development of all-solid-state Li-ion batteries.

[1] M.W. Swift and Y. Qi, Phys. Rev. Lett. 122, 167701 (2019)

[2] H.-K. Tian and Y. Qi, J. Electrochemical Society 164 (11), E3512-E3521

[3] H.-K. Tian, B. Xu, and Y. Qi Journal of Power Sources 392 (2018) 79–86

[4] H.-K. Tian, Z. Liu, Y. Ji, L.-Q. Chen, and Y. Qi, Chemistry of Materials 31 (2019) 7351-7359

+ Author for correspondence: yueqi@egr.msu.edu [mailto:yueqi@egr.msu.edu]

Author Index

Bold page numbers indicate presenter