2D Materials

Room A216 - Session 2D+EM+MI+NS-TuA

Properties of 2D Materials including Electronic, Magnetic, Mechanical, Optical, and Thermal Properties II

Moderator: Roland Wiesendanger, University of Hamburg, Germany

2:20pm **2D+EM+MI+NS-TuA-1 Boundary Conditions for a Continuum Model of Lateral Interfaces in Transition Metal Dichalcogenides**, ***Kaelyn Ferris,*** Ohio University

Tight-binding models of in-plane, lateral heterostructures of commensurate transition-metal dichalcogenides (TMD), such as MoS_2-WS_2 and $MoSe_2$-WSe_2 have demonstrated the appearance of laterally localized effective one-dimensional interfacial and edge states with unique features. These states lie within the band gap of the bulk structure and may provide a stable, tunable one-dimensional platform for possible use in exploring Majorana fermions, plasma excitations, and potential spintronics applications [1]. Motivated by the possible versatility of these modes in a variety of 2D systems, we now explore their appearance in continuum model descriptions of effective massive Dirac systems at low energy. We use different k*p models to characterize TMD nanoribbons and analyze proposals for the appropriate boundary conditions at lateral interfaces with various terminations. In particular we examine an *M*-Matrix approach [2] and envelope function approximation to obtain suitable boundary conditions.

[1] O. Avalos-Ovando et al., J. Phys.: Cond. Matt. **31**, 213001 (2019).

[2] C. G. Peterfalvi et al., Phys. Rev. B **92**, 245443 (2015).

2:40pm **2D+EM+MI+NS-TuA-2 Resolving the Structural and Electronic Properties of Graphene/Ge(110)**, ***Luca Camilli,*** Technical University of Denmark, Denmark; *M Galbiati,* Technical University of Denmark; *L Persichetti, M De Seta,* Università degli Studi Roma Tre, Italy; *F Fabbri,* Italian Institute of Technology, Italy; *A Scaparro,* Università degli Studi Roma Tre, Italy; *A Notargiacomo,* Centro Nazionale di Ricerca, Italy; *V Miseikis, C Coletti,* Italian Institute of Technology, Italy; *L Di Gaspare,* Università degli Studi Roma Tre, Italy

Unraveling the structural and electronic properties of the interface between graphene and conventional semiconductors is critical to enable novel graphene-based applications [1].

In this framework, the graphene/Ge(110) system has since last year received unprecedented attention [2-6]. Notably, graphene can be grown via chemical vapor deposition directly on the surface of germanium, similarly to the case of graphene grown on metals [7]. From a structural point of view, the graphene/Ge system is very dynamic, and the Ge surface has been shown by scanning tunneling microscopy (STM) studies to undergo a number of changes (i.e., reconstructions). However, the conclusions drawn in those studies do not always agree, probably also due to the strong dependence of the STM images on the applied voltage bias that makes comparison between different images rather difficult. In Ref. [6], for instance, the authors report three different surface reconstructions that are driven by thermal annealing, while the authors in Ref. [4] find only the unreconstructed surface and a (6x2) reconstruction, which again can reversibly change to unreconstructed surface after annealing at high temperature in hydrogen.

In this study, we aim at resolving the rich phase diagram of the Ge surface protected by graphene. We carry out annealing of the sample at different temperatures, and use a low-temperature STM to investigate the surface structure with atomic precision. At each stage, images at different applied biases are collected in order to allow a more straightforward comparison of the results.

Moreover, we perform electron energy loss spectroscopy (EELS) and scanning tunneling spectroscopy (STS) at temperature below 10 K to shed light on the electronic properties of the graphene/Ge interface, and to get more insights into their interaction.

Finally, we also show through a combination of STM and Raman spectroscopy that graphene can protect the germanium surface from oxidation even after continuous exposure to ambient conditions for more than 12 months, which is surprisingly a far more efficient protection than that offered by graphene on metals [8, 9].

References

[1] J.-H. Lee et al. Science 344, 286 (2014)

[2] G. Campbell et al. Physical Review Materials 2, 044004 (2018)

[3] J. Tesch et al. Nanoscale 10, 6068 (2018)

[4] D. Zhou et al. Journal of Physical Chemistry C 122, 21874 (2019)

[5] H.W. Kim et al. Journal of Physical Chemistry Letters 9, 7059 (2018)

[6] B. Kiraly et al. Applied Physics Letters 113, 213103 (2018)

[7] X. Li et al. Science 324, 5932 (2009)

[8]F. Zhou et al. ACS Nano 7, 6939 (2013)

[9] X. Zhang et al. Physical Chemistry Chemical Physics 18, 17081 (2016)

3:00pm **2D+EM+MI+NS-TuA-3 Array of Strain Induced Quantum Dots in Graphene**, ***Md Tareq Mahmud,*** *N Sandler,* Ohio University

Local Gaussian-shaped deformations induce strain fields that are represented by scalar and vector potentials in a continuum model description of electron dynamics in graphene. The ubiquitous strain changes the charge distribution in a very peculiar way, introducing a sublattice symmetry breaking, as has been reported in the literature. This feature can be exploited to design specific charge profiles by combining several deformations. Naturally, a combination of two or more is expected to introduce interference effects that can enhance charge accumulation in specific regions. We have investigated the effects of two overlapping deformations with different separations on the local density of states (LDOS). We showed that the overlap term can enhance the LDOS leading to stronger charge confinement in certain regions. Motivated by the work of Mason et. al (2018) we have extended these studies to a closed pack structure with a unit cell of 3 distinct deformations. This arrangement can be extended by symmetry to a lattice superstructure, thus creating a periodic array of confined charge regions, i.e, quantum dots. This array can be tailored by appropriately choosing the parameters of the deformations and their distances. The total charge distribution in these systems is similar to those observed in twisted bilayer systems, known as 'Moire patterns'. We discuss optimal tuning of deformations to control the physical properties of these graphene devices.

3:20pm **2D+EM+MI+NS-TuA-4 Ultrafast Spin and Charge Dynamics in Monolayer WSe_2-Graphene Heterostructure Devices**, ***Michael Newburger,*** *K Luo,* The Ohio State University; *K McCreary,* U.S. Naval Research Laboratory; *I Martin, E McCormick,* The Ohio State University; *B Jonker,* U.S. Naval Research Laboratory; *R Kawakami,* The Ohio State University

Monolayer transition metal dichalcogenides (TMDs) have attracted attention due to their long spin/valley lifetimes and ability to couple the helicity of light to spin/valley polarization. Additionally, a strength of TMDs lies in their ability to complement other materials, such as graphene, by acting as a means of optical spin injection or proximity coupling. Recently, multiple groups have demonstrated proximity mediated charge transfer and optical spin injection in TMD/graphene heterostructures. However, the spin transfer dynamics across a TMD/graphene interface remain largely unexplored.

Here we utilize time-resolved Kerr rotation (TRKR) microscopy to image the spatial dependence of spin/valley dynamics in monolayer WSe_2/graphene heterostructure devices. Spatial maps demonstrate long-lived spin/valley lifetimes on the bare WSe_2 but reveal a quenching of spin-valley signal at the WSe_2/graphene interfaces. Time delay scans show these interface lifetimes to be quenched up to 3 orders of magnitude in comparison to bare WSe_2. Furthermore, photoluminescence mapping exhibits quenching at the interfaces while photoconductivity is enhanced in these regions, demonstrating efficient charge transfer from WSe_2 to graphene. Consequently, we attribute the ultrafast spin/valley quenching to the transfer of spin information by conducted charge carriers.

4:20pm **2D+EM+MI+NS-TuA-7 Spatially Selective Enhancement of Photoluminescence in MoS by Exciton-Mediated Adsorption and Defect Passivation**, ***Saujan V. Sivaram,*** *A Hanbicki, M Rosenberger, G Jernigan, H Chuang, K McCreary, B Jonker,* U.S. Naval Research Laboratory

Monolayers of transition metal dichalcogenides (TMDs) are promising components for flexible optoelectronic devices due to their direct band gap and atomically thin nature. The photoluminescence (PL) from these materials is often strongly suppressed by non-radiative recombination mediated by mid-gap defect states. Here, we demonstrate up to a 200-fold increase in PL intensity from monolayer MoS_2 synthesized by chemical vapor deposition (CVD) by controlled exposure to laser light in ambient. This spatially resolved passivation treatment is air and vacuum stable. Regions unexposed to laser light remain dark in fluorescence despite continuous impingement of ambient gas molecules. A wavelength dependent study confirms that PL brightening is concomitant with exciton generation in the MoS_2; laser light below the optical band gap fails to

produce any enhancement in the PL. We highlight the photo-sensitive nature of the process by successfully brightening with a low power broadband white light source (< 10 nW). We decouple changes in absorption from defect passivation by examining the degree of circularly polarized PL. This measurement, which is independent of exciton generation, confirms that laser brightening reduces the rate of non-radiative recombination in the MoS_2. A series of gas exposure studies demonstrate a clear correlation between PL brightening and the presence of water. We propose that H_2O molecules passivate sulfur vacancies in the CVD-grown MoS_2, but require photo-generated excitons to overcome a large adsorption barrier. This work represents an important step in understanding the passivation of CVD-synthesized TMDs and demonstrates the interplay between adsorption and exciton generation.

This research was performed while S.V.S and M.R.R held a National Research Council fellowship and H.-J.C. held an American Society for Engineering Education fellowship at NRL.

4:40pm **2D+EM+MI+NS-TuA-8 Strained Graphene in the Quantum Hall Regime: Valley Splitting and Extra Conducting Channels**, ***Daiara Faria,*** Ohio University / Universidade do Estado do Rio de Janeiro*; C León,* Brigham Young University*; L Lima,* Universidade Rural do Rio de Janeiro, Brazil*; A Latgé,* Universidade Federal Fluminense, Brazil*; N Sandler,* Ohio University

The coupling between electronic and mechanical properties in 2D materials has become an important tool to control valleytronics. Graphene experiments have been reported with common deformations such as membrane bending that induces strain in the samples [1]. It has also been shown that strain affects charge distributions and graphene transport properties. Motivated by these responses, we have studied the effect of folds and wrinkles in graphene. New 'edge'-like states along the graphene folded region, that are valley polarized, were found and explored [2]. To take advantage of the existence of these new states, it would be desirable to separate their contribution from the continuum extended states that make graphene a semimetal.

Here we present a theoretical study of folds effects on a graphene membrane in the quantum Hall regime. We show that the addition of an external magnetic field allows the isolation of the valley polarized edge states in energy and in real space. Local density of state calculations in the deformation region predict the valley split peaks, as observed in recent experimental [3]. Using recursive Green's function method, we are able to reveal new extra conducting channels due to the "new edges" at the deformation region. These extra conducting channels could be detected in transport measurements.

A discussion is presented to bring attention on the role of the deformation parameters on the graphene quantum Hall regime and their relations with the magnetic lengths. With this in mind, we perform an analytic study based on the continuum (Dirac) description of electrons in graphene. In this model, the deformation is considered as a perturbation to the Landau Level states. The results show the existence of two different regimes, characterized by the ratio between the magnetic length and the deformation width ($\gamma = l_B/b$). For $\gamma<1$ the magnetic confinement allows the electrons to follow the strain potential profile. In this regime, the spatial separation between the polarized currents is larger. This could encourage the design of devices where contacts can efficiently detect these polarized currents.

[1] Y. Jiang et al., Nano Lett. 17, 2839 (2017).

[2] R. Carrillo-Bastos et al., PRB 94, 125422 (2016).

[3] S. Li, arXiv:1812.04344.

5:00pm **2D+EM+MI+NS-TuA-9 Unraveling the Novel Quantum Phenomena in Two-dimensional Materials using Transport and Photoemission Spectroscopy**, ***Jyoti Katoch,*** Carnegie Mellon University **INVITED**

The extreme surface sensitivity of two-dimensional (2D) materials provides an unprecedented opportunity to engineer the physical properties of these materials via changes to their surroundings, including substrate, adsorbates, defects, etc. In addition, 2D materials can be mechanically assembled layer-by-layer to form vertical or lateral heterostructures, making it possible to create new material properties merely by the choice of the constituting 2D layers and the relative twist angle between them. In this talk, I will discuss our recent transport [1] and photoemission [2, 3] results that shed light on the intricate relationship between controlled external perturbations, substrate, and electronic properties of 2D materials. I will show that the decoration of the 2D materials with adatoms, such as sub-lattice selective atomic hydrogenation of graphene and alkali metal doping of single layer WS_2 can be utilized to tailor electronic properties and induce novel quantum phenomena in 2D landscape.

[1] Katoch et. al., Physical Review Letters 121, 136801 (2018).

[2] Katoch et. al., Nature Physics 14, 355-359 (2018).

[3] Søren Ulstrup, et. al., arXiv:1904.06681 (2019).

5:40pm **2D+EM+MI+NS-TuA-11 Electronic Properties and Charge Density Wave Transition in Single-layer VSe_2**, ***Kien Nguyen-Cong,*** *P Neto, M Batzill, I Oleynik,* University of South Florida

Single-layer VSe_2 has been recently attracted attention due to experimental observations of ferromagnetism and charge density wave (CDW) transition. There are controversies from both theory and experiment concerning ferromagnetism in both bulk and single layer VSe_2.In addition, CDW transition in VSe_2 is not well understood. In this work, structural, electronic, magnetic and CDW properties of this system are investigated using first-principle calculations. The calculated electronic structure is compared with recent APPRES measurements and conclusions concerning its magnetic state are made. The calculated phonon spectra are used in investigation of CDW transition mechanism. Crystal structure of the CDW state is determined using the evolutionary crystal structure prediction combined with lattice dynamics.

6:00pm **2D+EM+MI+NS-TuA-12 Tunable Band Gap and Thermal Conductivity Measurements of Monolayer $MoSe_2$ by S Incorporation**, ***Shyama Rath,*** *V Singh,* University of Delhi, India

Monolayer $MoSe_2$ was grown on insulating SiO2/Si substrates by chemical vapor deposition. Scanning electron microscopy and optical contrast images were used to determine the domain size, morphology, and the number of layers. The crystallinity, and thickness of the synthesized domains were determined by Raman spectroscopy. The band gap was determined from Photoluminescence (PL) spectroscopy. The PL emission was absent for more than 4 layers, and the peak position varied from 1.48 eV for 4 layers to 1.55 eV in the monolayer limit. Sulphur incorporation was done to obtain MoS_xSe_{2-x} so as to obtain a further tunability of the bandgap. The band gap changes from 1.55 eV for monlayer $MoSe_2$ to 1.64 eV for monolayer $MoS_{0.32}Se_{0.68}$. Further, larger area domains were achieved in the alloy as compared to binary. The thermal conductivity of the monolayer $MoSe_2$ and MoS_xSe_{2-x} were determined from temperature-dependant Raman spectroscopy.

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