2D Materials Focus Topic
Room: 15 - Session 2D+MI-ThM

Novel Quantum Phenomena in 2D Materials

Moderator: Kai Xiao, Oak Ridge National Laboratory

8:00am **2D+MI-ThM1 Quantum Plasmonics with 2D Materials**, ***Dmitri Voronine***, University of South Florida

Quantum plasmonics effects were previously investigated in coupled metallic nanostructures with sub-nanometer gaps leading to large electron tunneling contributions. Two-dimensional transition metal dichalcogenides are promising materials with interesting optoelectronic, catalytic and sensing applications which may be integrated with plasmonic nanostructures and used in the quantum plasmonics regime. Their nanoscale optical characterization using tip-enhanced photoluminescence (TEPL) and tip-enhanced Raman scattering (TERS) spectroscopies provides detailed local structure-function information which is not available using far-field diffraction-limited techniques. Nanoscale optical imaging provides an improved understanding of the optoelectronic properties of edge states, defects and grain boundaries. Here we report nanoscale TEPL and TERS characterization of monolayer and few-layer 2D materials such as MoS2, WS2, MoSe2 and WSe2 and their alloys and heterostructures with subdiffraction spatial resolution due to the strong signal enhancement via surface plasmon confinement of the nano-size metallic tip. We investigate the limits of signal enhancement on various substrates by varying the tip-sample gap and reveal quantum plasmonic behavior for sub-nanometer gaps. We show that quantum plasmonics provides a new mechanism of the generation and control of excitons and trions in 2D materials via electron tunneling. We investigate various quantum plasmonics regimes with picometer-scale indentation control. These results may be used for improving the nano-optical properties of 2D materials and for designing novel quantum optoelectronic devices.

8:20am **2D+MI-ThM2 Investigation and Manipulation of One-Dimensional Charge Density Waves in MoS_2**, ***Wouter Jolie***, *C. Murray, J. Hall*, Institute of Physics II, University of Cologne, Germany, *F. Portner*, Institute for Theoretical Physics, University of Cologne, Germany, *B. Pielić*, Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Zagreb, Croatia, *N. Atodiresei*, Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany, *M. Kralj*, Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Zagreb, Croatia, *A. Rosch*, Institute for Theoretical Physics, University of Cologne, Germany, *C. Busse*, Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany, *T. Michely*, Institute of Physics II, University of Cologne, Germany

Grain boundaries in monolayer transition metal dichalcogenides (TMDC) are predicted to host one-dimensional metallic states embedded in an otherwise insulating layer. As was shown recently for $MoSe_2$ [1,2], these states may be electronically unstable, undergoing a Peierls transition which leads to a charge density wave (CDW) at low temperatures.

We investigate epitaxial monolayer-MoS_2 on graphene on Ir(111) with scanning tunneling microscopy and spectroscopy (STM/STS). We find a large bandgap in MoS_2 showing that it is well decoupled from the substrate. The MoS_2 islands feature long, straight, highly symmetric twin boundaries. Along these we measure a small bandgap together with periodic beatings in the local density of states, both characteristic of CDWs. We investigate different types of line defects in MoS_2 and find correspondingly different CDWs. These quasi-freestanding wires offer an opportunity to study the simple yet rich physics of CDWs, not often seen in true 1D form experimentally. Specifically, we investigate their properties based on symmetry analysis, the impact of point defects, temperature-dependence, phase-behavior and their response to doping.

[1] S. Barja, S. Wickenburg, Z.-F. Liu, Y. Zhang, H. Ryu, M.M. Ugeda, Z. Hussain, Z.-X. Shen, S.-K. Mo, E. Wong, M.B. Salmeron, F. Wang, M.F. Crommie, D.F. Ogletree, J.B. Neaton, A. Weber-Bargioni, *Nat. Phys.* **12**, 751-756 (2016)

[2] Y. Ma, H.C. Diaz, J. Avila, C. Chen, V. Kalappattil, R. Das, M.-H. Phan, T. Čadež, J.M.P. Carmelo, M.C. Asensio, M. Batzill, *Nat. Commun.* **8**, 14231 (2017)

8:40am **2D+MI-ThM3 Configuring Electronic States in an Atomically Precise Array of Quantum Boxes**, ***Seyedeh Fatemeh Mousavi***, *S. Nowakowska, A. Wäckerlin*, University of Basel, Switzerland, *I. Piquero-Zulaica*, Materials Physics Center, San Sebastián, Spain, *J. Nowakowski*, Paul Scherrer Institut (PSI), Switzerland, *S. Kawai*, University of Basel, Switzerland, *C. Wäckerlin*, Paul Scherrer Institut (PSI), Switzerland, *M. Matena, T. Nijs, S. Fatayer, O. Popova, A. Ahsan, T. Ivas, E. Meyer*, University of Basel, Switzerland, *M. Stöhr*, University of Groningen, Netherlands, *J.E. Ortega*, Materials Physics Center, San Sebastián, Spain, *J. Björk*, Linköping University, Sweden, *L.H. Gade*, Universität Heidelberg, Germany, *J. Lobo-Checa*, Universidad de Zaragoza, Spain, *T.A. Jung*, Paul Scherrer Institut (PSI), Switzerland

Quantum boxes (QBs) [1] have been arranged in extended 2D arrays by the self-assembled formation of a porous on-surface coordinated network [2]. Xe atoms were used as an adsorbate for their well-defined interaction with the surface state electrons of Cu(111), which is dominated by Pauli repulsion. The electronic states contained in these arrays can be configured by the localized perturbation by the targeted filling level of the individual QBs with Xe atoms after Xe repositioning, each quantum box exhibits maximal 12 filling levels, which incrementally perturb the quantum box state(s) via Pauli repulsion. It is shown that specific filling patterns of the network of the QBs which are coupled in an inherently precise way by self assembly [3] specifically perturb, and thus modify the localized and delocalized quantum box states (QBSs). In particular the energy levels of the QBSs is modulated also it is demonstrated that the inter-box coupling can be sustained or significantly weakened by an appropriate arrangement of empty and filled boxes. We gain unprecedented insight into the physics of interacting quantum states on the local level as well as in their cooperative interaction by using complementary scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission spectroscopy (ARPES) measurements. Our approach establishes that such self-assembled two-dimensional quantum box architectures may serve as nanoscale analog of breadboards that are commonly employed in electronic circuitry and guide towards the fabrication of quantum devices.

References

[1] S. Nowakowska et al., Nature Communications | 6:6071 | DOI: 10.1038/ncomms7071

[2] J. Lobo Checa et al., Science 325, 17, 300ff (2009)

[3] S. Nowakowska et al, small, 2016; DOI: 10.1002/smll.201600915..

9:00am **2D+MI-ThM4 A Quantum Berry Phase Switch in Circular Graphene Resonators**, ***Daniel Walkup****, *F. Ghahari, C. Gutierrez*, NIST/CNST, *J.F. Rodriquez-Nieva*, Harvard University, *Y. Zhao, J. Wyrick, F.D. Natterer, W.G. Cullen*, NIST/CNST, *K. Watanabe, T. Tanaguchi*, National Institute for Materials Science, Japan, *L.S. Levitov*, MIT, *N.B. Zhitenev, J.A. Stroscio*, NIST/CNST

In graphene and other 2D Dirac materials, the band structure has the property that momentum-space paths enclosing the Dirac point pick up a Berry phase of π. In a uniform magnetic field, this leads to a special quantization rule and an N=0 Landau level at the Dirac point. In a circular graphene resonator, weak magnetic fields can tune the quantized electron orbits between states with Berry phases of zero and π, leading to a discontinuous jump in the quantum energy level as a function of applied field. Here we report scanning tunneling microscopy and spectroscopy (STM/S) studies of circular resonators fabricated in p-n junction rings in graphene/hBN backgated devices. We observe direct signatures of a Berry-phase-induced switching of the resonator states measured with scanning tunneling spectroscopy as a function of magnetic field. The telltale signature is a sudden and large increase in the energy of angular-momentum states in the graphene p-n junction resonators when a small critical magnetic field is reached, in agreement with theoretical calculations of Dirac potential wells.

9:20am **2D+MI-ThM5 Nanostructured Graphene: A Platform for Fundamental Physics and Applications**, ***Antti-Pekka Jauho***, Technical University of Denmark, Denmark **INVITED**

Despite of its many wonderful properties, pristine graphene has one major drawback: being a semimetal it does not have a band gap, which complicates its applications in electronic devices. Many routes have been suggested to overcome this difficulty, such as cutting graphene into nanoribbons, using chemical methods or periodic gates, and - which is the paradigmatic example of this talk - by making regular nanoperforations, also known antidot lattices [1]. All these ideas work beautifully in theory, but realizing them in the lab

*** NSTD Postdoc Finalist**

is very difficult because fabrication steps inevitably induce disorder and other nonidealities, with potentially disasterous consequences for the intended device operation. In this talk I introduce these ideas and review the state-of-the –art both from the theoretical and the experimental points of view. I also introduce some new ideas, such as triangular antidots [2], and nanobubbles formed in graphene [3]. Our simulations, relying on advanced numerical techniques, show that it may be possible to generate very high quality spin- and valley polarized currents with these structures – something that has not yet been achieved in the lab. Importantly, our simulations involve millions of atoms which is necessary in order to address structures feasible in the lab.

[1] T. G. Pedersen et al., "Antidot lattices: designed defects and spin qubits", *Physical Review Letters,* vol. 100, 136804, April 2008

[2] S. S. Gregersen et al., "Nanostructured graphene for spintronics", *Phys. Rev. B.* vol 95, 121406(R), March 2017

[3] M. Settnes et al., "Graphene Nanobubbles as Valley Filters and Beam Splitters", *Phys. Rev. Lett.* vol. 117, 276801, December 2016

11:00am **2D+MI-ThM10 Anomalous Kondo Resonance Mediated by Graphene Nanoribbons**, ***Yang Li***, Ohio University and Argonne National Laboratory, *A. Ngo*, Argonne National Laboratory, *K.Z. Latt*, Ohio University, *B. Fisher*, Argonne National Laboratory, *S.W. Hla*, Argonne National Laboratory and Ohio University

Atomically precise graphene nanoribbons (AGNR) are formed by one dimensional graphene sheets of carbon atoms and they can exhibit semiconducting characteristics with varying bandgaps. For the device and sensor applications, it is important to explore AGNR heterostructures. Here, we form molecular heterostructures using magnetic molecules and on-surface synthesized AGNRs on a Au(111) surface. Then the electronic and spintronic properties of the AGNR-magnetic molecule-Au(111) heterostructures are investigated by using scanning tunneling microscopy, tunneling spectroscopy and atomic/molecular manipulation schemes at 5 K substrate temperature in an ultrahigh vacuum environment. Although the AGNRs on Au(111) surface have a semiconducting characteristic with a large bandgap, we discover the unexpected Kondo resonance on molecules adsorbed on AGNRs. Interestingly, the observed Kondo temperatures of the molecules appear the same as the ones adsorbed on AGNRs and Au(111) surface including the atomic scale differences due to adsorption site. The experimental results are explained by density functional theory and numerical renormalization group theory calculations. We acknowledge the support of DOE SISGR grant: DE-FG02-09ER16109.

11:20am **2D+MI-ThM11 Valley Photoluminescence Polarization in Monolayer WSe_2**, ***Aubrey Hanbicki***, *M. Currie*, Naval Research Laboratory, *G. Kioseoglou*, University of Crete, *A.L. Friedman*, *B.T. Jonker*, Naval Research Laboratory

Monolayer materials such as WS_2 or WSe_2 are direct gap semiconductors with degenerate, yet inequivalent *k*-points at *K* and *K'*. The valence band maxima for *K* and *K'* have spin states of opposite sense enabling one to selectively populate each valley independently with circularly polarized light. Subsequent valley populations can be determined via the polarization of emitted light. Optical emission is dominated by neutral and charged exciton (trion) features, and changes in emitted polarization provide insight into the fundamental processes of intervalley scattering. We measure the circularly polarized photoluminescence of WSe_2 monolayers as a function of excitation energy for both continuous-wave (cw) and pulsed laser excitation sources. Using cw excitation, the temperature dependence of the depolarization of the trion follows the same trend as that of the neutral exciton and involves collisional broadening. However, the initial polarization of the trion is nearly twice the polarization of the neutral exciton at low temperature. When a pulsed laser is used as the excitation source, the initial polarization of the neutral exciton increases and becomes very similar to the trion. We propose either an up-conversion process or screening from the instantaneously large carrier density generated by the pulsed excitation to explain these data. The difference in polarization behavior is linked to the different way energy is deposited in the system during these measurements. We also discuss changes in the photoluminescence induced by pulsed laser excitation.

This work was supported by core programs at NRL and the NRL Nanoscience Institute, and by the Air Force Office of Scientific Research #AOARD 14IOA018-134141.

11:40am **2D+MI-ThM12 Imaging Superconducting Topological Surface States in Non-centrosymmetric $PbTaSe_2$**, ***Tien-Ming Chuang***, Academia Sinica, Taiwan, Republic of China **INVITED**

The search for topological superconductors (TSCs) is one of the most exciting subjects in condensed matter physics. TSCs are characterized by a full superconducting gap in the bulk and topologically protected gapless surface (or edge) states. Within each vortex core of TSCs, there exist the zero energy Majorana bound states, which are predicted to exhibit non-Abelian statistics and to form the basis of the fault-tolerant quantum computation. So far, no stoichiometric bulk material exhibits the required topological surface states (TSSs) at E_F combined with fully gapped bulk superconductivity. Here, we use spectroscopic-imaging scanning tunneling microscopy to study the atomic and electronic structures of the non-centrosymmetric superconductor, PbTaSe2. Our results demonstrate PbTaSe2 as a promising candidate as a 2D TSC.

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