2D Materials
Room A226 - Session 2D+EM+MI+MN+NS+QS-TuM

Novel Quantum Phenomena
Moderator: Arend van der Zande, University of Illinois at Urbana Champaign

8:00am **2D+EM+MI+MN+NS+QS-TuM-1 Charge Density-Wave States in Single-Layer Transition-Metal Dichalcogenides***, **Phil King**,* University of St Andrews, UK **INVITED**

Control over materials thickness down to the single-atom scale has emerged as a powerful tuning parameter for manipulating not only the single-particle band structures of solids, but increasingly also their interacting electronic states and phases. A particularly attractive materials system in which to explore this is the transition-metal dichalcogenides, both because of their naturally-layered van der Waals structures as well as the wide variety of materials properties which they are known to host. Yet, how their interacting electronic states and phases evolve when thinned to the single-layer limit remains a key open question in many such systems. Here, we use angle-resolved photoemission to investigate the electronic structure and charge density wave (CDW) phases of monolayer $TiSe_2$, $TiTe_2$, and VSe_2. Three-dimensionality is a core feature of the electronic structure of all of these parent compounds, but we show how their CDW phases not only persist, but are strengthened, in the monolayer limit. In $TiSe_2$, we observe an orbital-selective CDW, necessarily without a k_z-selectivity in band hybridisation that is of key importance for the bulk instability,[1] while $TiTe_2$ is driven into a charge-ordered phase in the monolayer which is not stable in the bulk at all. In VSe_2, we show how the monolayer hosts a much stronger-coupling CDW instability than the bulk, which in turn drives a metal-insulator transition, removing a competing instability to ferromagnetism.[2] Together, these studies point to the delicate balance that can be realized between competing interacting states and phases in monolayer transition-metal dichalcogenides.

This work was performed in close collaboration with M.D. Watson, A. Rajan, J. Feng, D. Biswas, and colleagues from the Universities of St Andrews, Oxford, Keil, Diamond, Elettra, and SOLEIL.

[1]Watson *et al.*, Phys. Rev. Lett. 122 (2019) 076404.

[2]Feng *et al.,* Nano Lett. 18 (2018) 4493.

8:40am **2D+EM+MI+MN+NS+QS-TuM-3 Sublattice Symmetry Breaking and Kondo-effect Enhancement in Strained Graphene***, D Zhai,* Ohio University*; K Ingersent,* University of Florida*; S Ulloa, **Nancy Sandler**,* Ohio University

Kondo physics in doped monolayer graphene is predicted to exhibit unusual features due to the linear vanishing of the pristine material's density of states at the Dirac point. Despite several attempts, conclusive experimental observation of the phenomenon remains elusive. One likely obstacle to identification is a very small Kondo temperature scale *TK* in situations where the chemical potential lies near the Dirac point. We propose tailored mechanical deformations of monolayer graphene as a means of revealing unique fingerprints of the Kondo effect. Inhomogeneous strains are known to produce specific alternating changes in the local density of states (LDOS) away from the Dirac point that signal sublattice symmetry-breaking effects. Small LDOS changes can be amplified in an exponential increase or decrease of *TK* for magnetic impurities attached at different locations. We illustrate this behavior in two deformation geometries: a circular "bubble" and a long fold, both described by Gaussian displacement profiles. We calculate the LDOS changes for modest strains and analyze the relevant Anderson impurity model describing a magnetic atom adsorbed in either a "top-site" or a "hollow-site" configuration. Numerical renormalization-group solutions of the impurity model suggest that higher expected *TK* values, combined with distinctive spatial patterns under variation of the point of graphene attachment, make the top-site configuration the more promising for experimental observation of signatures of the Kondo effect. The strong strain sensitivity of *TK* may lift top-site Kondo physics into the range experimentally accessible using local probes such as scanning tunneling microscopy.

9:00am **2D+EM+MI+MN+NS+QS-TuM-4 Indirect Transition and Opposite Circular Polarization of Interlayer Exciton in a MoSe2 WSe2 van der Waals Heterostructure***, **Hsun-Jen Chuang**, A Hanbicki, M Rosenberger, C Hellberg, S Sivaram, K McCreary, I Mazin, B Jonker,* U.S. Naval Research Laboratory

An emerging class of heterostructures involves monolayer semiconductors such as many of the transition metal dichalcogenides (TMDs) which can be combined to form van der Waals heterostructures (vdWHs). One unique new optical property of heterostructure is an interlayer exciton (ILE), a spatially indirect, electron-hole pair with the electron in one TMD layer and the hole in the other. Here, we fabricated MoSe2/WSe2 hetero-bilayer encapsulated in h-BN with the alignment angle close to 60 degree between MoSe2 and WSe2. Followed by the state-of-the-art preparation techniques (Nano-squeegee) to ensure the optimal contact between the TMDs. The Strong ILE emission is observed with the emission energy around 1.35 eV at room temperature and resolve this emission into two distinct peaks (ILE1 and ILE2) separated by 24 meV at zero field at 5 K. Furthermore, we demonstrate that the two emission peaks have *opposite*circular polarizations with up to +20% for the ILE1 and -40% for ILE2 when excited by circularly polarized light. A*b initio* calculations provide an explanation of this unique and potentially useful property and indicate that it is a result of the indirect character of *both* electronictransitions. These peaks are *doubleindirect* excitons. *i.e.*indirect in both real and reciprocal space, split by relativistic effects.

This research was performed while H.-J.C. held an American Society for Engineering Education fellowship and M.R.R and S.V.S held a National Research Council fellowship at NRL. This work was supported by core programs at NRL and the NRL Nanoscience Institute. This work was also supported in part by a grant of computer time from the DoD High Performance Computing Modernization Program at the U.S. Army Research Laboratory Supercomputing Resource Center.

9:20am **2D+EM+MI+MN+NS+QS-TuM-5 Integrating 2D Magnet 1T-$MnSe_2$ with Topological Insulator Bi_2Se_3***, **Tiancong Zhu**,* The Ohio State University*; D O'Hara,* University of California, Riverside*; J Repicky, S Yu, M Zhu, B Noesges, T Liu, M Brenner, L Brillson, J Hwang, F Yang, J Gupta, R Kawakami,* The Ohio State University

Integrating two-dimensional(2D) magnet with topological insulator is an exciting topic. Other than the possible proximity induced magnetic ordering inside topological insulator, the 2D magnet/ topological insulator heterostructure can also lead to more efficient spin orbit torque switching, or the formation of magnetic skyrmions. The recent discovery of room temperature ferromagnetic ordering in 2D material MnSe and VSe further brings more potential in such heterostructure systems. In this talk, we report the synthesis and characterization of 2D magnet 1T-MnSe on topological insulator Bi Se . Monolayer of MnSe is grown on Bi Se with molecular beam epitaxy, and subsequently characterized with various techniques, including X-ray diffractometry (XRD), X-ray photoemission spectroscopy (XPS) and scanning tunneling microscopy (STM). STM measurement reveals the co-existence of monolayer a-MnSe(111) and 1T-$MnSe_2$ on Bi_2Se_3 surface. By performing spin-polarized STM measurement with Cr tip, we observed directly the magnetic signal from 1T-$MnSe_2$ on Bi_2Se_3. The growth of 1T-$MnSe_2$ on Bi_2Se_3 further leads to the MBE synthesis of magnetic topological insulator Bi_2MnSe_4, which also shows ferromagnetism down to the monolayer limit. The structural and magnetic characterization of the material will also be discussed in this talk.

9:40am **2D+EM+MI+MN+NS+QS-TuM-6 Effect of Exchange-correlation Functional and Structural Constraints on the Transition Temperature of Two- Dimensional Ferroelectrics***, **Shiva P. Poudel**, J Villanova, B Miller, A Pandit, S Barraza-Lopez,* University of Arkansas, Fayetteville

In this presentation, I will discuss two inconsistent models for obtaining the transition temperature (T_c) of two-dimensional (2D) ferroelectrics. It will be shown that the inconsistency arises from the choice of exchange-correlation functional and structural constraints [1-4] by obtaining T_c for a SnSe monolayer with PBE and vdW exchange-correlation functional, and with increased constraints. It has been found that vdW functional gives a larger T_c in comparison with PBE functional. Also, the increasing constraint raises T_c as well. Afterward, a complete analysis of the converged unit cell with seven different exchange-correlation functional will be provided. These results represent the most comprehensive theoretical benchmarks for these intriguing 2D ferroelectric materials.

This work was funded by an Early Career Grant from the DOE (Grant No. DE-SC0016139). Calculations were performed on Cori at the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-

AC02-05CH11231 and Arkansas High-Performance Computing Center's *trestles*, which is funded through the multiple National Science Foundation grants and the Arkansas Economic Development Commission.

References:

1. M. Mehboudi et al., Nano Lett. **16**, 1704 (2016).

2. M. Mehboudi, et al., Phys. Rev. Lett. **117**, 246802 (2016).

3. S. Barraza-Lopez, et al., PRB **97**, 024110 (2018).

4. R. Fei, et al., Phys. Rev. Lett. **117**, 097601 (2016).

11:00am **2D+EM+MI+MN+NS+QS-TuM-10 Sign-change Pairing Symmetry in Single Layer FeSe/$SrTiO_3$ Film***, **Huimin Zhang**,* West Virginia University*; Z Ge, M Weinert,* University of Wisconsin*; L Li,* West Virginia University

Single layer FeSe film epitaxially grown on $SrTiO_3$(001) substrate has drawn much interest for its novel interfacial effects, which have led to the highest superconducting temperature (T_C) to date amongst all Fe-based superconductors. While several paring states, such as sign-persevering s_{++}-wave, sign-changing nodeless *d*-wave and $s_{\pm}$-wave have been suggested, the pairing symmetry remains to be experimentally validated. Here we investigate the intrinsic impurity-induced in-gap bound states and quasiparticle interference (QPI) patterns in single layer FeSe/$SrTiO_3$ by scanning tunneling microscopy/spectroscopy. We observed bound states induced by nonmagnetic impurities, which strongly suggests a sign-changing order parameter. Through detailed analysis of the phase-sensitive QPI patterns, we further confirm that the order parameter indeed changes sign within the electron pockets. This identification of a sign change pairing symmetry in single layer FeSe/$SrTiO_3$ presents a critical step towards the understanding of its high T_c superconductivity.

11:20am **2D+EM+MI+MN+NS+QS-TuM-11 High Temperature Superconductivity in Epitaxial Single Layer $FeTe_{1-x}Se_x$/STO(001)***, **Qiang Zou**, Z Ge, C Yan, H Zhang, L Li,* West Virginia University

Single crystal FeTe exhibits a distinct long-range bicollinear antiferromagnetic order that can be suppressed by alloying with Se, where superconductivity emerges at a critical Se concentration of 0.3 with a T_C of 10 K. In this work, we show that this phase transition can be further modulated by reducing the thickness of $FeTe_{1-x}Se_x$, downto the single atomic layer limit. High quality single layer $FeTe_{1-x}Se_x$ films are grown on $SrTiO_3$(001) substrate by molecular beam epitaxy and characterized by scanning tunneling microscopy/spectroscopy and angle-resolved photoemission spectroscopy. We find the electronic properties are strongly dependent on the Se content. For x < 0.1, hole-like bands cross the Fermi level and form a hole-pocket at the Γ point with no states observed around the M point, indicating no superconductivity. With increasing Se content, the top of the valence bands moves away from the Fermi level, accompanied by a decrease in effective mass at the Γ point. For x > 0.1, the hole pocket at Γ point moves below the Fermi level, and an electron-pocket emerges at M point where a superconducting gap opens with a T_C of ~50 K. These findings and their implications for the emergence and stabilization of superconductivity in Fe-based superconductors at reduced dimensions will be presented at the meeting.

11:40am **2D+EM+MI+MN+NS+QS-TuM-12 The Observation of Majorana Zero Mode and Conductance Plateau in an Iron-based Superconductor***, **Hong-Jun Gao**,* Institute of Physics, Chinese Academy of Sciences, China **INVITED**

Majorana zero-modes (MZMs) are spatially-localized zero-energy fractional quasiparticles with non-Abelian braiding statistics that hold great promise for topological quantum computing. Recently, by using scanning tunneling microscopy/spectroscopy (STM/STS), a new breakthrough of Majorana zero mode (MZM) was achieved in a single material platform of high-T_c iron-based superconductors, $FeTe_{0.55}Se_{0.45}$, which combined advantages of simple material, high- T_c, and large ratio of Δ/E_F [1]. A detail STM/STS study of a $FeTe_{0.55}Se_{0.45}$ single crystal, also revealed the mechanism of two distinct classes of vortices present in this system, which directly tied with the presence or absence of zero-bias peak [2]. To further investigated the MZM, it is still needed to find a "smoking-gun" type of evidence for the existence of MZM, and a quantized conductance plateau is widely believed to be one of them. Here we report an observation of the Majorana conductance plateau in vortices on the iron superconductor $FeTe_{0.55}Se_{0.45}$ surface by using STM/STS [3]. We found that both extrinsic instrumental convoluted broadening and intrinsic quasiparticle poisoning can reduce the conductance plateau value. When extrinsic instrumental broadening is removed by deconvolution, the plateau is found to nearly reach a $2e^2/h$ quantized value. The direct observation of a conductance plateau on a single zero-mode in a vortex strongly supports the existence and protection of MZMs in this iron-based superconductor, which can serve as a single-material platform for Majorana braiding at relatively high temperature.

* In collaboration with, D.F. Wang[1,2], L.Y. Kong[1,2], P. Fan[1,2], H. Chen[1], S.Y. Zhu[1,2], W.Y. Liu[1,2], L. Cao[1,2], Y.J. Sun[1,2], S.X. Du[1,2,3], J. Schneeloch[4], R.D. Zhong[4], G.D. Gu[4], Liang Fu[5], Hong Ding[1,2,3].

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[1] D. F. Wang et al, *Science*.**362**, 333 (2008).

[2] L. Y. Kong et al, arXiv:1901.02293 (submitted to *Nature Physics* on November 19, 2018)

[2] S. Y. Zhu et al, arXiv: 1904.06124 (submitted to *Science* on February 15, 2019)

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