

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-TuM1 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.

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

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

9:00am **2D+EM+MI+MN+NS+QS-TuM4 Indirect Transition and Opposite Circular Polarization of Interlayer Exciton in a $\text{MoSe}_2/\text{WSe}_2$ van der Waals Heterostructure**, *Hsun-Jen Chuang*, A.T. Hanbicki, M.R. Rosenberger, C.S. Hellberg, S.V. Sivaram, K.M. McCreary, I.I. Mazin, B.T. 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 $\text{MoSe}_2/\text{WSe}_2$ hetero-bilayer encapsulated in h-BN with the alignment angle close to 60 degree between MoSe_2 and WSe_2 . 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. *Ab 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* electronic transitions. These peaks are *double indirect* 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-TuM5 Integrating 2D Magnet 1T-MnSe₂ with Topological Insulator Bi₂Se₃**, *Tiancong Zhu*, The Ohio State University; *D. O'Hara*, University of California, Riverside; *J.J. Repicky*, S. Yu, M. Zhu, B.A. Noesges, T. Liu, M. Brenner, L.J. Brillson, J. Hwang, F.Y. Yang, J.A. 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 Bi₂Se₃. Monolayer of MnSe is grown on Bi₂Se₃ 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-MnSe₂ on Bi₂Se₃ surface. By performing spin-polarized STM measurement with Cr tip, we observed directly the magnetic signal from 1T-MnSe₂ on Bi₂Se₃. The growth of 1T-MnSe₂ on Bi₂Se₃ further leads to the MBE synthesis of magnetic topological insulator Bi₂MnSe₄, 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-TuM6 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 *trellis*, 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-TuM10 Sign-change Pairing Symmetry in Single Layer $\text{FeSe}/\text{SrTiO}_3$ Film**, *Huimin Zhang*, West Virginia University; *Z. Ge*, M. Weinert, University of Wisconsin; *L.L. Li*, West Virginia University

Single layer FeSe film epitaxially grown on $\text{SrTiO}_3(001)$ 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 pairing 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 $\text{FeSe}/\text{SrTiO}_3$ 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 $\text{FeSe}/\text{SrTiO}_3$ presents a critical step towards the understanding of its high T_c superconductivity.

Tuesday Morning, October 22, 2019

11:20am **2D+EM+MI+MN+NS+QS-TuM11 High Temperature Superconductivity in Epitaxial Single Layer FeTe_{1-x}Se_x/STO(001)**, Qiang Zou, Z. Ge, C. Yan, H. Zhang, L.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, down to the single atomic layer limit. High quality single layer FeTe_{1-x}Se_x films are grown on SrTiO₃(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-TuM12 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 investigate 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. Chen¹, 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. Schneeloch⁴, R.D. Zhong⁴, G.D. Gu⁴, Liang Fu⁵, Hong Ding^{1,2,3}.

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[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)

Author Index

Bold page numbers indicate presenter

— B —

Barraza-Lopez, S.: 2D+EM+MI+MN+NS+QS-TuM6, **1**

Brenner, M.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

Brillson, L.J.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

— C —

Chuang, H.-J.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

— G —

Gao, H.-J.: 2D+EM+MI+MN+NS+QS-TuM12, **2**

Ge, Z.: 2D+EM+MI+MN+NS+QS-TuM10, **1**;
2D+EM+MI+MN+NS+QS-TuM11, **2**

Gupta, J.A.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

— H —

Hanbicki, A.T.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

Hellberg, C.S.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

Hwang, J.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

— J —

Jonker, B.T.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

— K —

Kawakami, R.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

King, P.D.C.: 2D+EM+MI+MN+NS+QS-TuM1, **1**

— L —

Li, L.L.: 2D+EM+MI+MN+NS+QS-TuM10, **1**;
2D+EM+MI+MN+NS+QS-TuM11, **2**

Liu, T.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

— M —

Mazin, I.I.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

McCreary, K.M.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

Miller, B.: 2D+EM+MI+MN+NS+QS-TuM6, **1**

— N —

Noesges, B.A.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

— O —

O'Hara, D.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

— P —

Pandit, A.: 2D+EM+MI+MN+NS+QS-TuM6, **1**

Poudel, S.: 2D+EM+MI+MN+NS+QS-TuM6, **1**

— R —

Repicky, J.J.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

Rosenberger, M.R.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

— S —

Sivaram, S.V.: 2D+EM+MI+MN+NS+QS-TuM4, **1**

— V —

Villanova, J.: 2D+EM+MI+MN+NS+QS-TuM6, **1**

— W —

Weinert, M.: 2D+EM+MI+MN+NS+QS-TuM10, **1**

— Y —

Yan, C.: 2D+EM+MI+MN+NS+QS-TuM11, **2**

Yang, F.Y.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

Yu, S.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

— Z —

Zhang, H.: 2D+EM+MI+MN+NS+QS-TuM10, **1**;
2D+EM+MI+MN+NS+QS-TuM11, **2**

Zhu, M.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

Zhu, T.: 2D+EM+MI+MN+NS+QS-TuM5, **1**

Zou, Q.: 2D+EM+MI+MN+NS+QS-TuM11, **2**